Data Evaluation Report on the aerobic biotransformation of chlormequat chloride in water-sediment system

PMRA Submission Number {.....} EPA MRID Number 46715227

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OECD Data Point:
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Test material:
Common name: Chlormequat chloride.
Chemical name:
IUPAC name: 2-Chloroethyltrimethylammonium chloride.
CAS name: 2-Chloro-N,N,N-trimethylethanammonium chloride salt.
CAS No: 999-81-5.
Synonyms: CYCOCEL.
SMILES string: CN(C)(C)CCCl.[Cl-] (ISIS v2.3/Universal SMILES).
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EXECUTIVE SUMMARY

The biotransformation of [ethyl-^{14}C]-labeled 2-chloro-N,N,N-trimethylethanammonium chloride salt (chlormequat chloride; radiochemical purity >98%) was studied in river water-loamy sand sediment (water pH 7.74-8.31, total organic carbon 1.7 mg/L; sediment pH 7.27, organic carbon 0.74%) and pond water-silt loam sediment (water pH 7.55-7.67, total organic carbon 1.9 mg/L; sediment pH 6.89, organic carbon 4.41%) systems from Switzerland for 105 days under aerobic conditions in darkness at 20 ± 2EC. Based on the water volume, [^{14}C]chlormequat chloride was applied at a rate of 0.468 mg a.i./L. The sediment:water ratios used were *ca.* 1:2-3 (200-240 g wet wt. sediment:530 mL water). This experiment was conducted in accordance with German BBA Guidelines for the Official Testing of Plant Protectants Part IV, §5-1 (1990) and in compliance with USEPA GLP standards. The test system consisted of glass metabolism flasks (1-L) attached to a continuous flow-through (humidified, CO_2-free air, *ca.* 60-80 mL/minute) system with traps for the collection of CO_2 (2N NaOH) and volatile organics (ethylene glycol, 2N H_2SO_4). Sediment and water were pre-incubated for 1 month, then following treatment, duplicate flasks of each system type were collected after 0, 0.25 (6 hours), 1, 2, 7, 14, 30, 61 and 105 days of incubation. Water layer samples were either analyzed directly using TLC or concentrated via rotary evaporation (*ca.* 45°C) under reduced pressure prior to TLC analysis. Sediment samples were sequentially extracted 1-3 times with methanol:acidified (pH 2) water (1:1, v:v), followed by 1-5 times with acidic (pH 2) water. Aliquots of the extracts were combined and concentrated using rotary evaporation (*ca.* 40°C) under reduced pressure prior to TLC analysis. Water layers, sediment extracts, extracted sediment and trapping solutions were analyzed for total radioactivity using LSC. Water layer samples and sediment extracts were analyzed for [^{14}C]chlormequat chloride and its transformation products by normal-phase, one-dimensional TLC analysis. The following unlabeled reference standards were used for identification purposes: choline-chloride and acetylcholine-chloride.

The test conditions outlined in the study appear to have been maintained throughout the 105-day incubations. Conditions were primarily moderately reducing in the water layers and reducing in the sediments of both systems, with redox potentials averaging +169 ± 46 mV and -119 ± 29 mV, respectively. In the water layers of both systems, mean dissolved oxygen levels and pH were 6.7 ± 1.1 mg/L and 8.13 ± 0.18, respectively.

Recovery of radiolabeled material averaged 99.0 ± 7.8 (range 78.6-107.9%) of the applied for the river water-sandy loam systems and 98.3 ± 10.7% (range 76.2-109.5%) for the pond water-silt loam systems. Although there were no consistent patterns of decline in recoveries for either system, the lowest recoveries did occur from the 14-day interval onward, with the study authors attributing low recoveries to extensive mineralization of parent [^{14}C]chlormequat chloride. Dissipation of [^{14}C]chlormequat chloride and partitioning of [^{14}C]residues between the water layers and sediment phases was similar for the two systems, with initial adsorption slightly faster for the sandy loam sediment as compared to the silt loam. One major TLC fraction (R_f 0.01-0.02) was isolated from the river water-sandy loam systems but was not further characterized. Several minor products were detected in both systems, with one tentatively identified as choline-chloride. $^{14}CO_2$ (identification not confirmed) was a major transformation product for both

systems totaling 64.1-69.9% and 54.1-57.1% of the applied at study termination for the river water-sandy loam and pond water-silt loam systems, respectively; [^{14}C]volatile organics were not detected at any sampling interval.

Non-linear half-lives of chlormequat chloride in both systems were 3-5 days in the water, 7-8 days in the sediment and 5-9 days in the total systems. **Linear half-lives** were 6 days in the water, 14-15 days in the sediment and 11-12 days in the total systems. **Observed DT50 values** for the river water-sandy loam systems were 2-7 days in the water layer and total system and 7-14 days in the sediment, and for the pond water-silt loam systems were 7-14 days, 14-30 days and 7-14 days for the water layer, sediment and total system, respectively.

In river water-sandy loam systems, [^{14}C]chlormequat chloride in the total system decreased from 105.4-105.7% of the applied at time 0 to 37.4-40.3% at 7 days, 4.4-9.0% at 14 days, 1.7-2.0% at 30 days and was 0.1-0.2% at 105 days. In the water layer, [^{14}C]chlormequat chloride decreased from 105.4-105.7% at time 0 to 59.7-63.9% at 2 days, then was 2.9-25.6% at 7 days and ≤0.5% thereafter. In the sediment, [^{14}C]chlormequat chloride increased from 6.9-11.2% at 6 hours to 30.3-34.4% at 2 days, then was 11.8-37.4% at 7 days decreasing to 4.0-8.5% at 14 days, 1.3-1.7% at 30 days and 0.1-0.2% at study termination. A polar transformation product (R_f 0.01-0.02) was detected at maximums of 1.8-2.3% (14 days), 5.5-11.1% (14 days) and 7.3-13.4% (14 days) of the applied in the water, sediment and total system, respectively, and was 0.4-0.6%, 0.6-0.8% and 1.0-1.4%, respectively, at study termination. Choline-chloride was detected at maximums of 0.2-0.3%, 0.8-1.7% and 1.0-2.0% in the water, sediment and total system, respectively. Two additional unidentified [^{14}C]fractions were each detected at ≤0.2% in the total system. Extractable sediment [^{14}C]residues increased from 6.9-11.2% of the applied at 6 hours to 30.3-34.4% at 2 days, then were 15.7-40.1% at 7 days decreasing to 0.9-1.2% at 105 days. Non-extractable [^{14}C]residues increased from 1.3-2.6% at time 0 to 37.5-49.0% at 30 days and were 26.2-27.7% at 105 study termination. Organic matter fractionation of 105-day extracted sediment, containing 27.7% of the applied, found 12.7%, 7.3% and 7.7% of the applied associated with the humins, fulvic acids and humic acids, respectively. Following application of [^{14}C]chlormequat chloride to the water layer, [^{14}C]residues partitioned from the water layer to the sediment with average distribution ratios (water:sediment) of 6:1 at day 6 hours, 2:1 at 1 day, 1:1 at 2 days, 1:13 at 7 days and were 1:≥22 thereafter.

In pond water-silt loam systems, [^{14}C]chlormequat chloride in the total system decreased from 106.1-108.1% at time 0 to 74.9-91.5% at 7 days, then was 18.4-19.5% at 14 days, 4.1-6.3% at 30 days and 0.1-0.6% at study termination. In the water layer, [^{14}C]chlormequat chloride decreased from 106.1-108.1% at time 0 to 40.6-55.3% at 7 days and was ≤0.6% thereafter. In the sediment, [^{14}C]chlormequat chloride increased from 3.5-3.6% at 6 hours to 34.3-36.2% at 7 days, then decreased to 17.8-19.3% at 14 days, 3.7-6.1% at 30 days and was 0.1-0.6% at 105 days. Choline-chloride was detected at maximums of 0.5%, 5.2% and 5.5% in the water, sediment and total system, respectively. A polar product (R_f 0.01-0.02) was detected at maximums of 2.8%, 4.0% and 4.8% of the applied in the water, sediment and total system, respectively, and one additional unidentified [^{14}C]fraction was each detected at ≤0.1% in the total system. Extractable sediment [^{14}C]residues increased from 3.5-3.6% of the applied at 6 hours to 36.7-38.8% at 7

days, then decreased to 1.1-2.0% at study termination. Non-extractable [^{14}C]residues increased from 1.0-1.4% at time 0 to 46.5-59.2% at 30 days, then decreased to 28.6-31.3% at 105 days. Organic matter fractionation of 105-day extracted sediment, containing 31.3% of the applied, found 19.9%, 4.9% and 6.6% of the applied associated with the humins, fulvic acids and humic acids, respectively. Following application of [^{14}C]chlormequat chloride to the water layer, distribution ratios (water:sediment) were 10:1 at 6 hours, 4:1 at 1 day, 2:1 at 2 days, 1:1 at 7 days and 1:≥24 thereafter.

Transformation pathways, proposed by the study authors and consistent with the transformation products detected, involved incorporation of residues into the sediment with subsequent mineralization to CO_2. Additionally, one minor transformation product detected in both systems was tentatively identified as choline-chloride.

Results Synopsis:

Test system used: River water-sandy loam sediment from Switzerland.

Linear half-life in water: 5.8 days ($r^2 = 0.6414$).
Linear half-life in sediment: 13.5 days ($r^2 = 0.8723$).
Linear half-life in the total system: 10.5 days ($r^2 = 0.8713$).

Non-linear half-life in water: 2.6 days ($r^2 = 0.9765$).
Non-linear half-life in sediment: 6.7 days ($r^2 = 0.8203$).
Non-linear half-life in total system: 4.9 days ($r^2 = 0.9803$).

Observed DT50 in water: 2-7 days.
Observed DT50 in sediment: 7-14 days.
Observed DT50 in total system: 2-7 days.

Major transformation products:
- CO_2 (maximum 69.9% of applied).
- Unidentified polar compound (R_f 0.01-0.02; maximum 11.1% and 13.4% in the sediment and total system).

Minor transformation products:
- Choline-chloride (maximum 2.0% in total system).

Test system used: Pond water-silt loam sediment from Switzerland.

Linear half-life in water: 5.7 days ($r^2 = 0.7020$).
Linear half-life in sediment: 14.5 days ($r^2 = 0.9031$).
Linear half-life in the total system: 11.8 days ($r^2 = 0.9217$).

Non-linear half-life in water: 4.6 days ($r^2 = 0.9733$).
Non-linear half-life in sediment: 7.9 days ($r^2 = 0.9898$).
Non-linear half-life in total system: 8.7 days ($r^2 = 0.9532$).

Observed DT50 in water: 2-7/7-14 days.
Observed DT50 in sediment: 14-30 days.
Observed DT50 in total system: 7-14 days.

Major transformation products:
CO_2 (maximum 57.1% of applied).
Minor transformation products:
Choline-chloride (maximum 5.5% in total system).
Unidentified polar product (R_f 0.01-0.02; maximum 4.8% in total system).

Study Acceptability: This study is classified as **supplemental**. No significant deviations from good scientific practices were noted. It was not certain that all major transformation products were identified. For the portion of this study conducted with the river water-sandy loam systems, one TLC fraction (R_f 0.01-0.02) that reached maximums of 11.1% and 13.4% of the applied in the sediment and total system, respectively, was not identified.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with German BBA Guidelines for the Official Testing of Plant Protectants Part IV, §5-1 (1990; pp. 19, 22). The following significant deviation from the objectives of USEPA Subdivision N Guideline §162-4 was noted:

> For the river water-sandy loam systems, one unidentified TLC fraction (R_f 0.01-0.02) was detected at maximums in one of the replicates of 11.1% and 13.4% of the applied in the sediment in the total system. Subdivision N guidelines require identification of all transformation products detected at ≥10% of the applied.

COMPLIANCE: This study was conducted in compliance with USEPA GLP Standards 40 CFR, Part 160 (1989); OECD Principles of GLP (1981) and GLP in Switzerland - Procedures and Principles (1986, p. 19). Signed and dated Data Confidentiality, GLP and Quality Assurance statements were provided (pp. 2-5, 7).

A. MATERIALS:

1. Test Material [Ethyl-^{14}C]-labeled 2-chloro-N,N,N-trimethylethanammonium chloride salt (chlormequat chloride, p. 24).

Chemical Structure: See DER Attachment 1.

Description:		Technical; physical state not reported.
Purity:	Radiochemical purity:	>98% (pp. 24, 41; Figures 11-13, pp. 90-92).
	Lot/Batch No.	93211.
	Analytical purity:	Not reported.
	Specific activity:	94.6 µCi/mg (15.00 mCi/mmol, p. 24).
	Location of the radiolabel:	At the two ethyl carbons (p. 24).
Storage conditions of test chemical:		Radiolabelled test substance was stored frozen (temperature not specified) in darkness (p. 24).

Physico-chemical properties of chlormequat chloride:

Parameter	Value	Comment
Molecular weight	158.1 g/mol.	
Molecular formula	$C_5H_{13}Cl_2N$.	
Water Solubility	10^6 mg/L.	At 20°C.
pH	5-7.	At 20°C.
Physical state	White to yellowish, liquid.	
Vapor Pressure/Volatility	Not reported.	
UV Absorption	Not reported.	
Pka	Not reported.	
K_{ow}/log K_{ow}	Not reported.	
Stability of compound at room temperature	Not reported.	

Data obtained from p. 23 of the study report and p. 21 of MRID 46715225.

2. Water-sediment collection, storage and properties

Table 1: Description of water-sediment collection and storage.

Description		River	Pond
Geographic location.		Rhine, Mumpf Zeltplatz, Aargau/Switzerland.	Weiherhof-Tal, Ormalingen, Baselland/Switzerland.
Pesticide use history at the collection sites		Not reported.	
Collection date		August 10, 1993.	
Collection procedures for:	Water:	Water collected with a plastic container (not further described) and sediment collected with a shovel *ca.* 1-2 m from shore.	
	Sediment:		
Sampling depth for:	Water:	Sampled to 10- to 30-cm depth.	
	Sediment:	Upper 5- to 10-cm layer of sediment collected.	
Storage conditions		Water and sediment were transported in sealed containers to the test facility and stored at room temperature until sieved (interval not specified). After sieving, the water-sediment systems were stored at 4°C until preparation of the test flasks.	
Storage length		Six days after collection, water-sediment systems were prepared for a 1-month pre-incubation (acclimation) phase.	
Preparation	Water:	0.2-mm sieved.	
	Sediment:	2.0-mm sieved.	

Data obtained from p. 26; Tables 4-5, pp. 54-55 of the study report.

Table 2: Properties of the waters; determined at time of collection, except where noted.

Property		**Rhine River**		**Weiherhof-Tal Pond**	
Temperature (°C)	Surface	20.0		12.7	
	5 cm above sediment	20.0		11.8	
pH	Surface	8.31		7.67	
	5 cm above sediment	7.74		7.55	
Redox potential (mV)[1]		Initial	Final	Initial	Final
	Surface	+211	+180, +181, +185, +177	+102	+139, +184, +177, +173
	5 cm above sediment	+193		+38	
Oxygen concentration (mg/L)[1]		Initial	Final	Initial	Final
	Surface	7.8	7.2, 7.6, 7.6, 6.8	6.9	8.2, 6.7, 7.0, 4.8
	5 cm above sediment	7.4		4.8	
Dissolved organic carbon (%)		Not reported.			
Total organic carbon (mg/L)[2]		Initial	Final	Initial	Final
		1.7	13.9	1.9	16.5
Hardness (°dH)		11		18.5	
Electrical conductivity		Not reported.			
Biomass (mg microbial C/100 g or CFU or other)		Not reported.			

1 Initial measured at time of collection (Table 2, p. 52). Final measured in untreated and treated systems at 105 days posttreatment (Tables 6-7, pp. 56-59).
2 Determined at test facility.
Data obtained from Table 2, p. 52; Tables 6-7, pp. 56-59 of the study report.

Table 3: Properties of the sediments.

Property	Rhine River		Weiherhof-Tal Pond	
Soil texture	Loamy sand.		Silt loam.	
%sand (2000-50 Φm):	61.0		37.7	
%silt (50-2 Φm):	32.3		59.6	
%clay (<2 Φm):	6.7		2.7	
pH (In KCl)	7.27		6.89	
Organic carbon (%)	0.74		4.41	
Organic matter (%)[1]	1.27		7.59	
CEC (mVal N/100 g dry wt.)	8.7		8.9	
Redox potential (mV)[2]	Initial	Final	Initial	Final
	-154	-184, -211, -178, -158	-78	-136, -120, -131, -183
Bulk density (g/cm^3)	Not reported.			
Dry mass (kg dry wt./kg fresh wt.)	Initial	Final	Initial	Final
	0.6	0.6	0.3	0.3
Biomass (mg microbial C/100 g dry wt.)[3]	Initial	Final	Initial	Final
	79.2	69.1	325.9	223.6

1 Percent organic matter determined by primary reviewer using the following formula: organic matter (%) = organic carbon (%) x 1.72.
2 Initial measured at time of collection (Table 3, p. 53). Final measured in untreated and treated systems at 105 days posttreatment (Table 6, p. 57; Table 7, p. 59).
3 Initial at start of study and Final determined in untreated control sediment after 160 days of incubation.
Data obtained from Table 3, p. 53; Table 6, p. 57; Table 7, p. 59 of the study report.

B. EXPERIMENTAL DESIGN:

1. Preliminary experiments: No preliminary experiments were reported.

2. Experimental conditions:

Table 4: Study design.

Parameter		Rhine River	Weiherhof-Tal Pond
Duration of the test		105 days.	
Water:			
Filtered/unfiltered water:		Filtered.	
Type and size of filter used, if any:		0.2-mm sieve.	
Amount of sediment and water per treatment	Water:	530 mL; *ca.* 6-cm depth.	
	Sediment:	240 g wet wt.; *ca.* 2-cm depth.	200 g wet wt.; *ca.* 2-cm depth.

Parameter		Rhine River		Weiherhof-Tal Pond	
Water/sediment ratio		*ca.* 2.2:1 (mL:g wet wt.).		*ca.* 2.7:1 (mL:g wet wt.).	
Application rates (mg a.i./L)	Nominal:	0.468 mg a.i./L.			
	Actual:	0.468 mg a.i./L (248 µg a.i./530 mL).			
Control conditions, if used		No sterile controls were used.			
No. of replications	Control, if used:	No sterile controls were used.			
	Treated:	Per system type, twenty nonsterile systems were treated with [^{14}C]chlormequat chloride; eighteen for duplicate flasks at each sampling interval plus two reserves.			
Test apparatus (type/material/volume):		1-L, glass, metabolism flasks; inner diameter 10.6 cm.			
Details of traps for CO_2 and organic volatile, if any:		Up to 28 days posttreatment: 2N NaOH (one trap, 50 mL) to trap CO_2. Ethylene glycol (one trap, 50 mL) to trap organic volatiles. After 28 days: 2N NaOH (one trap, 50 mL) to trap CO_2. Ethylene glycol (one trap, 50 mL) and 2N H_2SO_4 (one trap, 50 mL) to trap organic volatiles.			
If no traps were used, is the system closed?		Volatiles traps were used with a continuous air-flow atmosphere.			
Identity and concentration of co-solvent		No co-solvent was used; test substance was dissolved in water.			
Test material application method	Volume of the test solution used/treatment:	980 µL.			
	Application method (eg: mixed/not mixed):	Test solution applied drop-wise via Hamilton syringe.			
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.			
Biomass (mg microbial C/100 g, CFU or other) of controls:		Initial	Final	Initial	Final
	Water:	No sterile controls were used.			
	Sediment:				
Biomass (mg microbial C/100 g, CFU or other) of treated:		Initial	Final	Initial	Final
	Water:	Treated systems were not analyzed for biomass.			
	Sediment:				
Experimental conditions:	Temperature (°C):	20 ± 2°C.			
	Continuous darkness (Yes/No):	Yes.			

Parameter	Rhine River	Weiherhof-Tal Pond
Other details, if any	Per system type, four untreated nonsterile water-sediment systems were prepared and incubated to monitor system parameters and for biomass determinations. The maximum recommended field application rate was reported as 1.4 kg a.i./ha). The application rate of 0.468 mg a.i./L was reported as equivalent to 1.4 kg a.i./ha.	

Data were obtained from pp. 20, 26, 28-30, 49, and Scheme 1, p. 76 of the study report.

3. Aerobic conditions: Water and sediment were combined in the metabolism flasks and maintained at 20 ± 2EC in darkness for 1 month prior to treatment (p. 28; Tables 4-5, pp. 54-55). Prior to and following treatment, humidified, CO_2-free air was continuously flushed (*ca.* 60-80 mL/minute) through the flask headspace, and the water layer was gently agitated via a suspended magnetic stirrer without disturbing the sediment (p. 28; Scheme 1, p. 76). In Rhine river water-sandy loam systems at day 0 posttreatment, redox potentials and dissolved oxygen in the water layers were +161 mV and 6.8-7.3 mg/L, respectively, with redox potentials in the sediment of -140 to -122 mV (treated systems only; Table 6, pp. 56-57). In Weiherhof-Tal pond water-silt loam systems at day 0, redox potentials and dissolved oxygen in the water layers were +162 to +163 mV and 5.7-5.9 mg/L, respectively, and redox potentials in the sediment were -99 to -95 mV (treated systems only; Table 7, pp. 58-59).

4. Supplementary experiments: No supplementary experiments were described.

5. Sampling:

Table 5: Sampling details.

Criteria	Both systems
Sampling intervals	0, 0.25 (6 hours), 1, 2, 7, 14, 30, 61 and 105 days.
Sampling method	Duplicate systems (flasks) were collected at each interval.
Method of collection of CO_2 and organic volatile compounds	Volatiles trapping solutions were collected and/or replaced at each sampling interval and/or weekly following treatment.
Sampling intervals/times for: Sterility check, if sterile controls are used: Redox potential, dissolved oxygen and pH in water layer and redox potential in sediment:	 No sterile controls were used. Measured at each sampling interval.
Sample storage before analysis	Water layers and sediment were separated the day of collection. No information regarding storage of water, sediment and/or sample extracts was provided.
Other observation, if any	None.

Data were obtained from pp. 28, 30-31; Tables 6-7, pp. 56-59 of the study report.

C. ANALYTICAL METHODS:

Separation of the sediment and water: The water layer was drawn off the sediment via a glass pipette and aliquots (1 mL, replicates not specified) were analyzed for total radioactivity by LSC (pp. 31-32).

Extraction/clean up/concentration methods: Water layer samples were either analyzed directly (200 µL) using TLC or concentrated via rotary evaporation (*ca.* 45°C) under reduced pressure prior to TLC analysis (p. 31).

Sediment samples were sequentially extracted 1-3 times with methanol:acidified (pH 2) water (1:1, v:v), followed by 1-5 times with acidic (pH 2) water; extraction solvent volumes were *ca.* 2 mL solvent/g wet wt. sediment (p. 31; Scheme 2, p. 77). Each extraction was done via shaker (*ca.* 250 strokes/minute) for *ca.* 30 minutes; subsequent separation of sediment and extract was not described. Aliquots (volumes not reported) of the extracts were combined and concentrated using rotary evaporation (*ca.* 40°C) under reduced pressure prior to TLC analysis.

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the water layers, sediment extracts, extracted sediment and volatile trapping solutions (Table 9, p. 61; Table 11, p. 63).

Determination of non-extractable residues: Extracted sediment was air-dried and homogenized in a mortar, then triplicate aliquots (up to 2.114 g) were analyzed for total radioactivity by LSC following combustion (pp. 31-32).

To separate non-extractable [^{14}C]residues into humin, humic acid and fulvic acid fractions, extracted 105-day sediments (aliquot size not specified) were further extracted with 0.5M NaOH; extraction solvent volume, extraction method and method to separate sediment and extract were not reported (p. 31). The extract was acidified to *ca.* pH 1, with the resulting precipitate (humic acids) removed by centrifugation. Analysis methods used to determine total radioactivity associated with the remaining supernatant (fulvic acids), precipitate (humic acids) and extracted soil (humin) were not reported.

Determination of volatile residues: Aliquots (0.5 mL, replicates not reported) of the NaOH trapping solutions were diluted with water (3.0-4.0 mL), then combined with scintillation solution (10 mL) and analyzed for total radioactivity by LSC, while aliquots (1 mL) of the ethylene glycol trapping solutions were combined directly with scintillation solution (10 mL) for LSC analysis (p. 32). Analysis of H_2SO_4 trapping solutions was not described.

Derivatization method, if used: A derivatization method was not employed.

Identification and quantification of parent compound: Water layer and sediment extract samples were analyzed using one-dimensional TLC on normal-phase cellulose plates developed with either 1-butanol:acetic acid:water (40:10:50, v:v:v; SS 1), 1-butanol:formic acid:water

(70:20:10, v:v:v; SS 2) or 1-butanol:ethanol:acetic acid:water (80:20:10:30, v:v:v:v; SS 3); on aluminum oxide plates developed with n-pentanol:water:formic acid (12:7:5, v:v:v, SS 4); and on silica gel plates (Merck 60 F254) developed with either ethanol:water:6N ammonium hydroxide (60:30:10, v:v:v; SS 5), chloroform:methanol (2:1, v:v; SS 6), or acetic acid:acetone:32% HCl (85:10:4, v:v; SS 7; p. 33). Solvent systems SS 3 and SS 4 were reported as used for routine analyses. Following development, areas of radioactivity were detected and quantified using a Berthold LB 2842 TLC Linear Analyser (p. 34). Parent [^{14}C]chlormequat chloride was identified by co-chromatography with and comparison to the Rf value of unlabeled reference standard (p. 34; Figures 14-21, pp. 93-100). To visualize unlabeled reference standard cellulose plates were sprayed with 1% phosphormolybdic acid in ethanol:chloroform (1:1, v:v), washed with water for 10 minutes, then stained with 1% tin chloride solution in 3N HCl (p. 33). To visualize unlabeled reference standard on aluminum oxide and silica gel plates the plates were sprayed with 1% molybdophosphoric acid in ethanol:chloroform (1:1, v:v), then placed in water for 1-2 minutes (p. 34).

Identification and quantification of transformation products: Transformation products were separated, quantified and identified using TLC as described for the parent compound (pp. 33-34; Figures 14-21, pp. 93-100).

To analyze water layers for dissolved $^{14}CO_2$, aliquots (up to 5 mL) were combined with saturated barium hydroxide solution (5 mL), with the resulting precipitate removed by centrifugation (*ca.* 2,500 rpm; p. 32). An aliquot (1.0 mL) of the supernatant was diluted with water (4 mL), then combined with scintillation solution (10 mL) and analyzed for total radioactivity by LSC.

Table 6: Reference compounds available for identifying transformation products of chlormequat chloride.

Applicant code	Chemical Name	Purity	Lot/Batch No.
Ref. A	Choline chloride	99%	--[1]
Ref. B	Acetylcholine chloride	98%	--

1 Information not provided.
Data obtained from p. 25 of the study report.

Detection limits (LOD, LOQ) for the parent compound: Limits of detection (LODs) for LSC analyses were reported as 0.10 ppb for 1-mL sediment extract samples and 1 g sediment combustions and <0.1 ppb for 10 mL water and sediment extract samples and 1.5 g sediment combustions (p. 38).

Detection limits (LOD, LOQ) for the parent compound: LODs and LOQs were the same as for the parent compound.

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: During the 105-day incubations, conditions for both systems were primarily moderately reducing (-50 to +200 mV) in the water layers and reducing (-200 to -50 mV) in the sediments. In river water-sandy loam sediment systems, average redox potentials in the water and sediment were +170 ± 44 mV (range +54 to +209 mV) and -131 ± 34 mV (-211 to -74 mV), respectively, with dissolved oxygen and pH levels of 6.5 ± 1.1 mg/L (3.5-7.8 mg/L) and 8.21 ± 0.14 (8.04-8.51), respectively, in the water (Table 6, pp. 56-57; DER Attachment 2). In pond water-silt loam sediment systems, average redox potentials in the water and sediment were +169 ± 48 mV (+42 to +210 mV) and -106 ± 13 mV (-136 to -83 mV), respectively, with dissolved oxygen and pH levels of 6.9 ± 1.0 mg/L (4.6-8.2 mg/L) and 8.05 ± 0.19 (7.46-8.36), respectively, in the water (Table 7, pp. 58-59; DER Attachment 2). Incubation temperatures were reportedly maintained at 20 ± 2EC during the study (p. 20); however, no supporting documentation was provided.

B. MATERIAL BALANCE: Overall recoveries of radiolabeled material averaged 99.0 ± 7.8% (range 78.6-107.9%, n = 18) of the applied for the river water-sandy loam systems and 98.3 ± 10.7% (range 76.2-109.5%, n = 18) for the pond water-silt loam systems (DER Attachment 2). Although there were no consistent patterns of decline in recoveries for either system, the lowest recoveries did occur from the 14-day interval onward, with the study authors attributing low recoveries to excessive mineralization of parent [^{14}C]chlormequat chloride (p. 42).

Partitioning of [^{14}C]residues between the water layers and sediment phases was similar for the two systems, with initial adsorption slightly faster for the sandy loam sediment as compared to the silt loam (DER Attachment 2). Following application of [^{14}C]chlormequat chloride to the water layer, [^{14}C]residues in the river water-sandy loam systems partitioned from the water layer to the sediment with average (n = 2) distribution ratios (water:sediment) of 6:1 at day 6 hours (0.25 day), 2:1 at 1 day, 1:1 at 2 days, 1:13 at 7 days and were 1:≥22 at 14-105 days. Distribution ratios for the pond water-silt loam systems were 10:1 at 6 hours, 4:1 at 1 day, 2:1 at 2 days, 1:1 at 7 days and 1:≥24 at 14-105 days.

Table 7: Biotransformation of [^{14}C]chlormequat chloride, expressed as percentage of applied radioactivity (mean ± s.d.[1], n = 2), in Swiss river water-sandy loam sediment under aerobic conditions.

Compound		Sampling times (days)								
		0	0.25[2]	1	2	7	14	30	61	105
Chlormequat-Cl	Water	105.6 ± 0.1	85.4 ± 6.2	73.1 ± 0.3	61.8 ± 2.1	14.3 ± 11.4	0.5 ± 0.1	0.4 ± 0.1	0.3, n.d.[3]	n.d.
	Sediment	n.a.[4]	9.1 ± 2.1	22.8 ± 0.3	32.4 ± 2.0	24.6 ± 12.8	6.3 ± 2.3	1.5 ± 0.2	0.5 ± 0.1	0.2 ± 0.1
	System	105.6 ± 0.1	94.4 ± 4.1	95.9 ± 0.1	94.1 ± 0.0	38.9 ± 1.4	6.7 ± 2.3	1.9 ± 0.2	0.6 ± 0.2	0.2 ± 0.1
RW1/RS1[5] (R_f 0.97 in SS3, 0.34/0.50 in SS4)	Water	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2 ± 0.0	n.d., 0.1	n.d.
	Sediment	n.a.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d., <0.1	<0.1, n.d.
	System	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2 ± 0.0	n.d., 0.1	<0.1, n.d.
RW2/RS2[5] (R_f 0.61 in SS3, 0.27/0.34 in SS4)	Water	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2 ± 0.0	n.d.	n.d.
	Sediment	n.a.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d., <0.1	n.d.	n.d.
	System	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2 ± 0.0	n.d.	n.d.
RW3/RS3[6] (R_f 0.44 in SS3, 0.13 in SS4)	Water	n.d.	n.d., 3.4	n.d.	n.d.	n.d.	n.d.	0.3 ± 0.1	n.d.	n.d.
	Sediment	n.a.	n.d.	n.d.	n.d.	n.d.	n.d.	1.3 ± 0.5	n.d.	0.2 ± 0.0
	System	n.d.	n.d., 3.4	n.d.	n.d.	n.d.	n.d.	1.5 ± 0.5	n.d., <0.1	0.2 ± 0.0
RW4/RS4[5] (R_f 0.01-0.02 in SS3, SS4)	Water	n.d.	1.7 ± 0.1	n.d.	n.d.	0.1, n.d.	2.1 ± 0.3	1.3 ± 0.2	1.3 ± 0.0	0.5 ± 0.1
	Sediment	n.a.	n.d.	n.d.	n.d.	3.3 ± 0.6	8.3 ± 2.8	1.5 ± 1.2	1.5 ± 0.1	0.7 ± 0.1
	System	n.d.	1.7 ± 0.1	n.d.	n.d.	3.4 ± 0.6	10.4 ± 3.1	2.8 ± 1.4	2.8 ± 0.0	1.2 ± 0.2
CO_2		n.a.	<0.1	0.1 ± 0.0	0.2 ± 0.1	18.9 ± 8.0	27.5 ± 7.7	46.8 ± 3.0	61.7 ± 3.8	67.0 ± 2.9
Volatile organics		n.a.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Extractable sediment residues		n.a.	9.1 ± 2.1	22.8 ± 0.3	32.4 ± 2.0	27.9 ± 12.2	14.6 ± 5.1	4.4 ± 1.5	1.9 ± 0.1	1.1 ± 0.2
Non-extractable sediment residues		2.0 ± 0.7	7.8 ± 1.5	7.7 ± 1.2	10.6 ± 0.3	34.2 ± 3.3	39.6 ± 3.0	43.3 ± 5.8	33.0 ± 2.3	27.0 ± 0.8
Total recovery	Water	105.6 ± 0.1	88.7 ± 4.4	73.1 ± 0.3	61.8 ± 2.1	14.3 ± 11.3	2.5 ± 0.3	2.2 ± 0.2	1.4 ± 0.0	0.5 ± 0.1
	Sediment	2.0 ± 0.7	16.8 ± 3.6	30.4 ± 1.4	42.9 ± 2.3	62.1 ± 8.9	54.2 ± 2.0	47.6 ± 4.3	34.9 ± 2.4	28.0 ± 0.9
	System	107.5 ± 0.5	105.5 ± 0.8	103.5 ± 1.1	104.9 ± 0.2	95.3 ± 5.6	84.1 ± 5.5	96.7 ± 7.0	98.0 ± 1.4	95.5 ± 1.9

Data obtained from Table 9, p. 61, Tables 13-14, pp. 65-66, Table 16, p. 68 of the study report and DER Attachment 2.

1 Reviewer's Comment No. 1.

2 Six hours.

3 Not detected.

4 Not analyzed.

5 Unidentified.

6 Tentatively identified as choline-chloride.

Table 8: Biotransformation of [^{14}C]chlormequat chloride, expressed as percentage of applied radioactivity (mean ± s.d.[1], n = 2), in Swiss pond water-silt loam sediment under aerobic conditions.

Compound		Sampling times (days)								
		0	0.25[2]	1	2	7	14	30	61	105
Chlormequat-Cl	Water	107.1 ± 1.0	98.1 ± 0.1	84.4 ± 1.9	73.5 ± 0.1	48.0 ± 7.3	0.4 ± 0.2	0.3 ± 0.2	0.2 ± 0.1	n.d.[3]
	Sediment	n.a.[4]	3.6 ± 0.1	13.3 ± 0.8	25.3 ± 1.0	35.3 ± 1.0	18.6 ± 0.8	4.9 ± 1.2	2.4 ± 1.2	0.4 ± 0.3
	System	107.1 ± 1.0	101.6 ± 0.1	97.7 ± 1.1	98.8 ± 1.0	83.2 ± 8.3	19.0 ± 0.5	5.2 ± 1.1	2.5 ± 1.1	0.4 ± 0.3
PW1/PS1[5] (R_f 0.98 in SS3, 0.3/0.5 in SS4)	Water	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1, <0.1	n.d.	n.d.
	Sediment	n.a.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1, n.d.	n.d.
	System	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1, <0.1	0.1, n.d.	n.d.
PW2/PS2[6] (R_f 0.49 in SS3, 0.13/0.18 in SS4)	Water	n.d.	n.d.	n.d.	n.d.	n.d.	n.d., 0.5	0.2 ± 0.1	0.1 ± 0.0	n.d.
	Sediment	n.a.	n.d.	n.d.	n.d.	n.d.	n.d.	3.2 ± 2.1	0.8 ± 0.1	0.4 ± 0.3
	System	n.d.	n.d.	n.d.	n.d.	n.d.	n.d., 0.5	3.4 ± 2.2	0.9 ± 0.1	0.4 ± 0.3
PW3/PS3[5] (R_f 0.01-0.02 in SS3, SS4)	Water	n.d.	n.d.	n.d.	1.8 ± 1.1	2.1 ± 0.4	1.7 ± 0.1	0.6 ± 0.0	0.2 ± 0.0	0.1 ± 0.0
	Sediment	n.a.	n.d.	n.d.	n.d.	n.d., 2.3	1.7 ± 0.1	2.5 ± 1.6	0.6 ± 0.0	0.8 ± 0.2
	System	n.d.	n.d.	n.d.	1.8 ± 1.1	3.3 ± 1.6	3.4 ± 0.1	3.1 ± 1.6	0.8 ± 0.1	0.9 ± 0.2
CO_2		n.a.	<0.1	0.1, <0.1	0.1 ± 0.0	1.9 ± 1.4	26.0 ± 0.8	33.7 ± 1.4	42.8 ± 7.9	55.6 ± 1.5
Volatile organics		n.a.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Extractable sediment residues		n.a.	3.6 ± 0.1	13.6 ± 0.5	25.3 ± 1.0	37.8 ± 1.0	20.2 ± 0.8	10.5 ± 2.4	3.7 ± 1.1	1.6 ± 0.5
Non-extractable sediment residues		1.2 ± 0.2	5.9 ± 0.0	9.1 ± 0.5	5.6 ± 0.1	13.3 ± 4.0	37.1 ± 0.3	52.9 ± 6.4	35.3 ± 0.6	30.0 ± 1.3
Total recovery	Water	107.1 ± 1.0	98.1 ± 0.1	84.4 ± 1.9	75.3 ± 1.2	50.1 ± 7.0	2.4 ± 0.0	1.2 ± 0.3	0.5 ± 0.0	0.1 ± 0.0
	Sediment	1.2 ± 0.2	9.5 ± 0.1	22.6 ± 1.1	30.9 ± 1.1	51.0 ± 2.9	57.3 ± 0.5	63.3 ± 8.7	39.0 ± 1.7	31.5 ± 1.8
	System	108.3 ± 1.2	107.5 ± 0.2	107.0 ± 0.8	106.2 ± 0.0	102.8 ± 2.7	85.6 ± 0.3	98.2 ± 10.3	82.3 ± 6.1	87.3 ± 0.3

Data obtained from Table 11, p. 63, Tables 18-19, pp. 70-71, Table 21, p. 73 of the study report and DER Attachment 2

1 Reviewer's Comment No. 1.

2 Six hours.

3 Not analyzed.

4 Not analyzed.

5 Unidentified.

6 Tentatively identified as choline-chloride.

C. TRANSFORMATION OF PARENT COMPOUND: Dissipation of [^{14}C]chlormequat chloride was similar and fairly rapid in both systems, yet, based on observed DT50 values, slightly faster in the pond water-silt loam sediment systems as compared to the river water-sandy loam sediment systems. In river water-sandy loam systems, [^{14}C]chlormequat chloride in the total system decreased from 105.4-105.7% of the applied at time 0 to 37.4-40.3% at 7 days, 4.4-9.0% at 14 days, 1.7-2.0% at 30 days and was 0.1-0.2% at 105 days (DER Attachment 2). In the water layer, [^{14}C]chlormequat chloride decreased from 105.4-105.7% at time 0 to 59.7-63.9% at 2 days, then was 2.9-25.6% at 7 days and ≤0.5% thereafter. In the sediment, [^{14}C]chlormequat chloride increased from 6.9-11.2% at 6 hours to 30.3-34.4% at 2 days, then was 11.8-37.4% at 7 days decreasing to 4.0-8.5% at 14 days, 1.3-1.7% at 30 days and 0.1-0.2% at 105 days.

In pond water-silt loam systems, [^{14}C]chlormequat chloride in the total system decreased from 106.1-108.1% at time 0 to 74.9-91.5% at 7 days, 18.4-19.5% at 14 days, 4.1-6.3% at 30 days and was 0.1-0.6% at 105 days (DER Attachment 2). In the water layer, [^{14}C]chlormequat chloride decreased from 106.1-108.1% at time 0 to 40.6-55.3% at 7 days, then was ≤0.6% thereafter. In the sediment, [^{14}C]chlormequat chloride increased from 3.5-3.6% at 6 hours to 34.3-36.2% at 7 days, then decreased to 17.8-19.3% at 14 days, 3.7-6.1% at 30 days and was 0.1-0.6% at 105 days.

Half-Life/DT50/DT90: Dissipation of chlormequat chloride appeared to be best described by nonlinear analysis (SigmaPlot v 8), with half-life values of 3, 7 and 5 days in the water (using 0- to 61-day intervals), sediment (2-105 days) and total system (all intervals), respectively, of the river water-sandy loam systems, and 5, 8 and 9 days in the water (0-61 days), sediment (7-105 days) and total system (all intervals), respectively, of the pond water-silt loam systems. Based on first order regression analysis (Excel 2000), the linear half-lives of chlormequat chloride were 6, 14 and 11 days in the water, sediment and total system, respectively, of the river water-sandy loam systems, and 6, 15 and 12 days, respectively, for the pond water-silt loam systems. Observed DT50 values were 2-7 days for the water and total system and 7-14 days for the sediment of the river water-sandy loam systems, and 2-7/7-14, 14-30 and 7-14 days for the water, sediment and total system, respectively, of the pond water-silt loam systems.

Based on nonlinear analysis (kinetic models of Timme, G., *et al.*), the study authors calculated DT50 values for chlormequat chloride of 0.5 days in the water layers of both systems, 0.9 days in the total river water-sandy loam systems and 6.6 days in the total pond water-silt loam systems.

Half-lives/DT50/DT90

Phase		Half-life/DT50[1] (days)	First order linear regression equation	r^2	DT50[2] (days)	DT90[2] (days)
Rhine river water-sandy loam sediment systems						
Water	Linear/natural log	5.8	y = -0.1196x + 3.6454	0.6414	--	--
	Nonlinear/normal	2.6	--	0.9765	0.5	5.4
	Observed DT50	2-7	--	--	--	--
Sediment	Linear/natural log	13.5	y = -0.0513x + 2.8603	0.8723	--	--
	Nonlinear/normal	6.7	--	0.8203	--	--
	Observed DT50	7-14	--	--	--	--
System	Linear/natural log	10.5	y = -0.0661x + 4.0420	0.8713	--	--
	Nonlinear/normal	4.9	--	0.9803	0.9	10.4
	Observed DT50	2-7	--	--	--	--
Weiherhof-Tal pond water-silt loam sediment systems						
Water	Linear/natural log	5.7	y = -0.1213x + 3.9002	0.7020	--	--
	Nonlinear/normal	4.6	--	0.9733	0.5	5.3
	Observed DT50	2-7/7-14	--	--	--	--
Sediment	Linear/natural log	14.5	y = -0.0480x + 3.5513	0.9031	--	--
	Nonlinear/normal	7.9	--	0.9898	--	--
	Observed DT50	14-30	--	--	--	--
System	Linear/natural log	11.8	y = -0.0590x + 4.4274	0.9217	--	--
	Nonlinear/normal	8.7	--	0.9532	6.6	21.9
	Observed DT50	7-14	--	--	--	--

1 Determined by the primary reviewer using Excel 2000 (linear) and Sigmaplot v 8.0 (nonlinear), and individual sample data obtained from Table 13A, p. 65; Table 18A, p. 70 of the study report (DER Attachment 2).
2 Determined by the study authors using 1st order and 1st order with respect to square root of time kinetic models of Timme, G. *et al.* (pp. 39-40, 48, 50; Table 23, p. 75; Figures 9-10, pp. 88-89).

TRANSFORMATION PRODUCTS: One major nonvolatile transformation product was detected in the river water-sandy loam systems, but not identified; with no major products detected in the pond water-silt loam systems. Several minor products were detected in both systems, with one, RW3/RS3 or PW2/PS2, tentatively identified as choline-chloride via TLC co-chromatography with reference standard (p. 46; Table 14, p. 66; Table 16, p. 68; Table 19, p. 71; Table 21, p. 73; Reviewer's Comment No. 2).

In river water-sandy loam systems, RW4/RS4 (polar fraction, R_f 0.01-0.02) was detected at maximums of 2.3% (14 days), 11.1% (14 days) and 13.4% (14 days) of the applied in the water, sediment and total system, respectively, and was 0.4-0.6%, 0.6-0.8% and 1.0-1.4%, respectively, at 105 days (DER Attachment 2). Choline-chloride (RW3/RS3) was detected at maximums of 0.3%, 1.7% and 2.0% in the water, sediment and total system, respectively. Two additional unidentified [^{14}C]fractions, RW1/RS1 and RW2/RS2 were each detected at ≤0.2% in the total system at any sampling interval.

In pond water-silt loam systems, PW3/PS3 (polar fraction, R_f 0.01-0.02) was detected at maximums of 2.8%, 4.0% and 4.8% of the applied in the water, sediment and total system, respectively (DER Attachment 2). Choline-chloride (PW2/PS2) was detected at maximums of 0.5%, 5.2% and 5.5% in the water, sediment and total system, respectively. One additional unidentified [^{14}C]fraction, PW1/PS1 was each detected at ≤0.1% in the total system at any sampling interval.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: For the sandy loam sediment, extractable sediment [^{14}C]residues increased from 6.9-11.2% of the applied at 6 hours to 30.3-34.4% at 2 days, then were 15.7-40.1% at 7 days decreasing to 0.9-1.2% at 105 days (Table 9, p. 61; DER Attachment 2). Non-extractable [^{14}C]residues increased from 1.3-2.6% at time 0 to 37.5-49.0% at 30 days, then decreased to 26.2-27.7% at 105 days. Organic matter fractionation of 105-day extracted sediment, containing 27.7% of the applied, found 12.7%, 7.3% and 7.7% of the applied associated with the humins, fulvic acids and humic acids, respectively (p. 47).

For the silt loam sediment, extractable sediment [^{14}C]residues increased from 3.5-3.6% of the applied at 6 hours to 36.7-38.8% at 7 days, then decreased to 1.1-2.0% at 105 days (Table 11, p. 63; DER Attachment 2). Non-extractable [^{14}C]residues increased from 1.0-1.4% at time 0 to 46.5-59.2% at 30 days, then decreased to 28.6-31.3% at 105 days. Organic matter fractionation of 105-day extracted sediment, containing 31.3% of the applied, found 19.9%, 4.9% and 6.6% of the applied associated with the humins, fulvic acids and humic acids, respectively (p. 47).

VOLATILIZATION: At study termination (105 days), volatilized $^{14}CO_2$ (identification not confirmed) totaled 64.1-69.9% and 54.1-57.1% of the applied radioactivity, for the river water-sandy loam and pond water-silt loam systems, respectively, with volatile [^{14}C]organic compounds not detected at any sampling interval for both systems (Table 9, p. 61; Table 11, p. 63; DER Attachment 2).

The study authors reported that barium hydroxide precipitation detected a "high amount" of dissolved $^{14}CO_2$ in the water layers of the river water-sandy loam systems, with dissolved $^{14}CO_2$ comprising 84% and 78% of the sample radioactivity in 14- and 105-day water samples, respectively from the pond water-silt loam systems (p. 44).

TRANSFORMATION PATHWAY: The transformation pathways proposed by the study authors for the dissipation of chlormequat chloride under aerobic aquatic conditions involve significant incorporation of residues into the sediment with subsequent mineralization to CO_2 (p. 49; Scheme 4, p. 79). In this study, one minor transformation product detected in both systems was tentatively identified as choline-chloride.

Table 9: Chemical names and CAS numbers for the transformation products of chlormequat chloride.

Applicant's Code/Name	CAS No.	Chemical Name	Chemical formula	MW (g/mol)	Smiles String
--	--	Choline-chloride	--	--	--

Data obtained from pp. 46-47 of the study report.

D. SUPPLEMENTARY STUDY- RESULTS: No supplementary experiments were described.

III. STUDY DEFICIENCIES

It was not certain that all major transformation products were identified. In the river water-sandy loam system, one unidentified TLC fraction, RW4/RS4, was isolated at maximums in one of the replicates of 11.1% of the applied from the sediment and 13.4% from the total system. This TLC area comprised 4.8% of the applied in the pond water-silt loam total system. The study authors did not conduct additional analyses to determine if this area consisted of one or several polar compounds. Subdivision N guidelines require identification of all transformation products detected at ≥10% of the applied.

IV. REVIEWER'S COMMENTS

1. Mean results and standard deviations presented in this review were determined by the primary reviewer using Microsoft Excel 2000 (9.0.2720) software (DER Attachment 2). Standard deviations were determined using the "biased" or "n" method which determines the standard deviation of the entire sample population. The mean results reported by the study authors (Table 9, p. 61; Table 11, p. 63; Tables 13-14, pp. 65-66; Table 16, p. 68; Tables 18-19, pp. 70-71; Table 21, p. 73) were verified by the primary reviewer and there was consistent agreement (within ± 0.1% of applied) between the study authors' reported mean values and those determined by the primary reviewer (DER Attachment 2).

2. The study authors reported that transformation product RW3/RS3 and PW2/PS2 was identified as choline-chloride via TLC co-chromatography with reference standard and also referred to as Ref. B (pp. 46-47). However, in other sections of the study text, Ref. B refers to the reference standard acetylcholine-chloride (p. 34; Table 1, p. 51). The study authors must clarify which is correct.

3. **Observed DT50 values for total residues.**

Phase	River water-sandy loam sediment		Pond water-silt loam sediment	
	Parent + nonvolatile transformation products	Total [^{14}C]residues[1]	Parent + nonvolatile transformation products	Total [^{14}C]residues[1]
Water	2-7 days	2-7 days	*ca.* 7 days	7-14 days
Sediment	7-14 days	*ca.* 105 days	14-30 days	*ca.* 105 days
Total system	2-7 days	30-61 days	7-14 days	61-105 days

1 All [^{14}C]residues other than volatilized $^{14}CO_2$.
Data obtained from DER Attachment 2.

V. REFERENCES

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2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

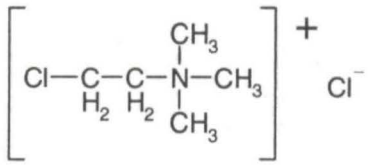
4. Wolfe, N., *et al.* 1990. Abiotic transformations in water, sediments and soil. *In* Pesticides in the Soil Environment, Soil Science Society of America, pp. 103-110.

Attachment 1: Structures of Parent Compound and Transformation Products

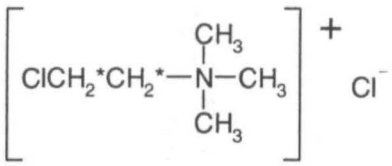
Chlormequat chloride [Cycocel]

IUPAC Name: 2-Chloroethyltrimethylammonium chloride.
CAS Name: 2-Chloro-N,N,N-trimethylethanaminium chloride.
CAS Number: 999-81-5.
SMILES String: CN(C)(C)CCCl.[Cl-] (ISIS v2.3/Universal SMILES).
ClCCN(Cl)(C)(C)C (EPI Suite, v3.12).

Unlabeled



[^{14}C]chlormequat chloride

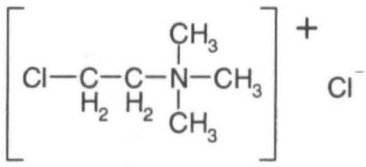


* = Position of radiolabel.

Identified Compounds

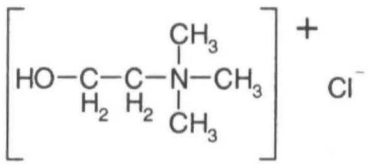
Chlormequat chloride [Cycocel]

IUPAC Name: 2-Chloroethyltrimethylammonium chloride.
CAS Name: 2-Chloro-N,N,N-trimethylethanaminium chloride.
CAS Number: 999-81-5.
SMILES String: CN(C)(C)CCCl.[Cl-] (ISIS v2.3/Universal SMILES).
ClCCN(Cl)(C)(C)C (EPI Suite, v3.12).



Choline chloride

IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.



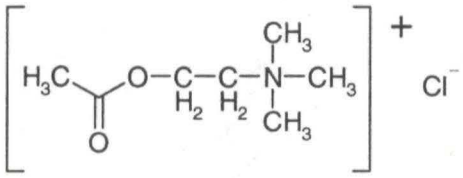
Carbon Dioxide

IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.

Unidentified Reference Compounds

Acetylcholine chloride

IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.



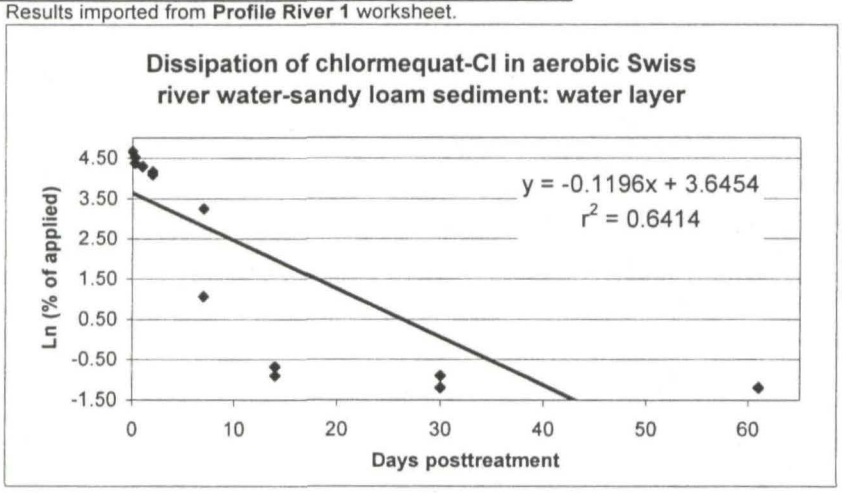
Attachment 2: Excel and SigmaPlot Spreadsheets

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Rhine river water-sandy loam sediment.
Half-life determination for water layer.
Half-life (days) 5.8 (0- to 61-day data)

	Chlormequat-chloride	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	105.4	4.657762636
0	105.7	4.660604893
0.25	91.6	4.517431272
0.25	79.2	4.371976299
1	72.8	4.287715955
1	73.4	4.295923936
2	59.7	4.08933202
2	63.9	4.157319361
7	2.9	1.064710737
7	25.6	3.242592351
14	0.5	-0.693147181
14	0.4	-0.916290732
30	0.4	-0.916290732
30	0.3	-1.203972804
61	0.3	-1.203972804
61		#NUM!
105		#NUM!
105		#NUM!

Results imported from **Profile River 1** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.800851699
R Square	0.641363444
Adjusted R Square	0.613776017
Standard Error	1.589181025
Observations	15

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	58.71373949	58.714	23.24839628	0.0003336
Residual	13	32.83145229	2.5255		
Total	14	91.54519177			

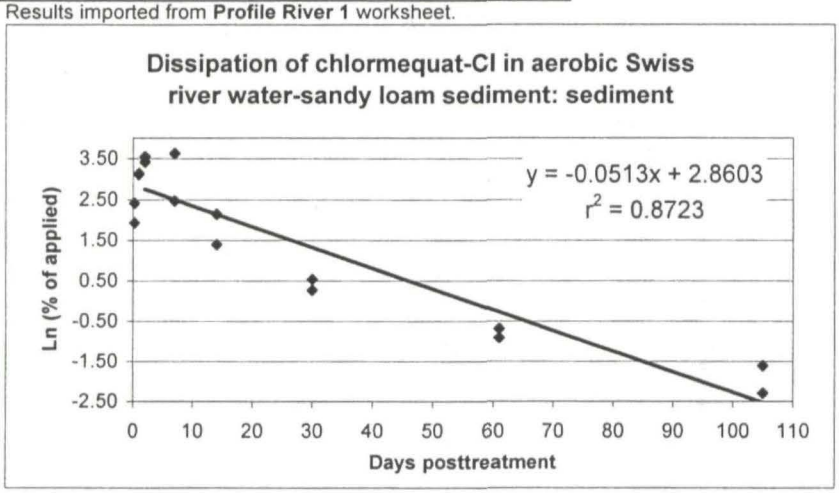
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.645409792	0.496899992	7.3363	5.69537E-06	2.5719228	4.7188968	2.57192283	4.718896754
X Variable 1	-0.119583786	0.024801377	-4.822	0.00033364	-0.173164	-0.0660037	-0.17316389	-0.06600368

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Rhine river water-sandy loam sediment.
Half-life determination for sediment.
Half-life (days) 13.5 (2- to 105-day data)

	Chlormequat-chloride	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	0.0	#NUM!
0	0.0	#NUM!
0.25	6.9	1.931521412
0.25	11.2	2.415913778
1	23.0	3.135494216
1	22.5	3.113515309
2	34.4	3.538056564
2	30.3	3.411147713
7	37.4	3.621670704
7	11.8	2.468099531
14	8.5	2.140066163
14	4.0	1.386294361
30	1.3	0.262364264
30	1.7	0.530628251
61	0.5	-0.693147181
61	0.4	-0.916290732
105	0.1	-2.302585093
105	0.2	-1.609437912

Results imported from **Profile River 1** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.933949256
R Square	0.872261213
Adjusted R Square	0.859487335
Standard Error	0.780996022
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	41.65061493	41.651	68.28475795	8.856E-06
Residual	10	6.099547862	0.61		
Total	11	47.75016279			

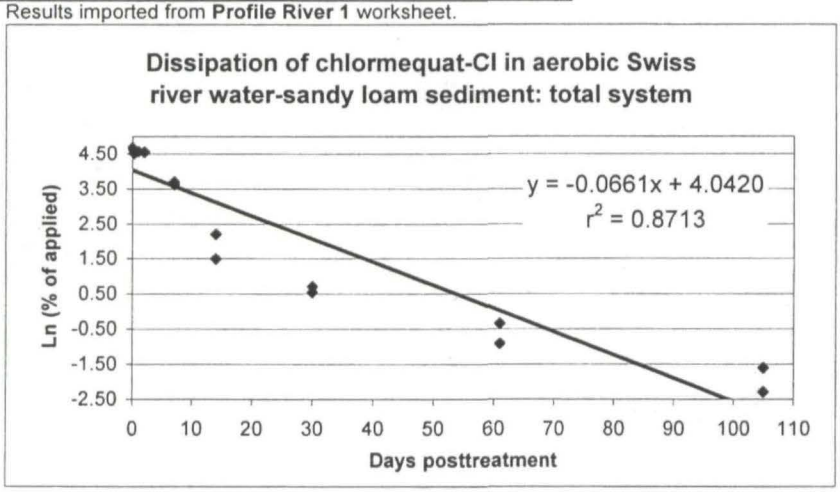
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.860251153	0.319767037	8.9448	4.37326E-06	2.1477657	3.5727366	2.14776567	3.572736635
X Variable 1	-0.051338236	0.006212681	-8.263	8.85563E-06	-0.065181	-0.0374955	-0.06518095	-0.03749552

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Rhine river water-sandy loam sediment.
Half-life determination for total system.
Half-life (days) 10.5 (0- to 105-day data)

	Chlormequat-chloride	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	105.4	4.657762636
0	105.7	4.660604893
0.25	98.4	4.589040804
0.25	90.3	4.50313746
1	95.8	4.562262685
1	95.9	4.563305982
2	94.1	4.544358047
2	94.1	4.544358047
7	40.3	3.696351469
7	37.4	3.621670704
14	9.0	2.197224577
14	4.4	1.481604541
30	1.7	0.530628251
30	2.0	0.693147181
61	0.7	-0.356674944
61	0.4	-0.916290732
105	0.1	-2.302585093
105	0.2	-1.609437912

Results imported from **Profile River 1** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.933409377
R Square	0.871253066
Adjusted R Square	0.863206382
Standard Error	0.920127546
Observations	18

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	91.66920597	91.669	108.2748037	1.576E-08
Residual	16	13.5461552	0.8466		
Total	17	105.2153612			

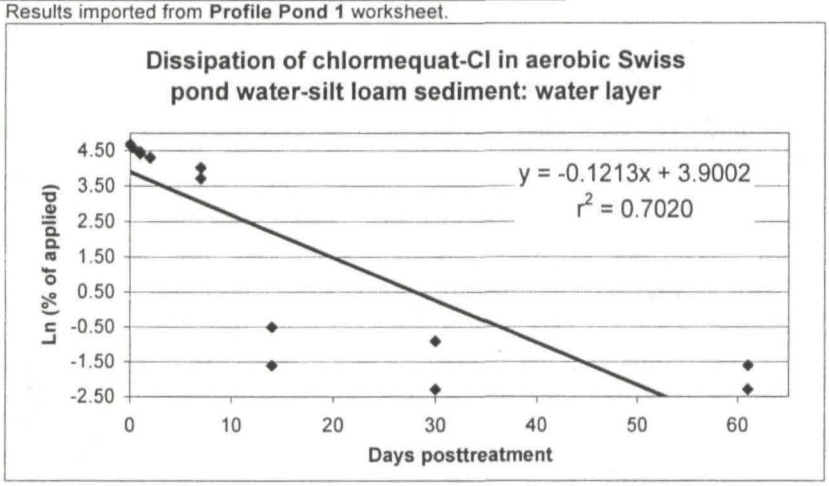
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.041987009	0.266769831	15.152	6.57066E-11	3.4764604	4.6075137	3.47646036	4.60751366
X Variable 1	-0.066050619	0.006347653	-10.41	1.5755E-08	-0.079507	-0.0525942	-0.07950704	-0.0525942

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Weiherhof-Tal pond water-silt loam sediment.
Half-life determination for water layer.
Half-life (days) 5.7 (0- to 61-day data)

	Chlormequat-chloride	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	108.1	4.683056725
0	106.1	4.664382046
0.25	97.9	4.58394655
0.25	98.2	4.587006215
1	86.3	4.457829598
1	82.5	4.412798293
2	73.4	4.295923936
2	73.6	4.298645026
7	55.3	4.012772909
7	40.6	3.703768067
14	0.6	-0.510825624
14	0.2	-1.609437912
30	0.4	-0.916290732
30	0.1	-2.302585093
61	0.2	-1.609437912
61	0.1	-2.302585093
105	0.0	#NUM!
105	0.0	#NUM!

Results imported from **Profile Pond 1** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.837834586
R Square	0.701966794
Adjusted R Square	0.680678708
Standard Error	1.692449613
Observations	16

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	94.45206235	94.452	32.97463138	5.092E-05
Residual	14	40.10139971	2.8644		
Total	15	134.5534621			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.900245687	0.521152578	7.4839	2.95017E-06	2.7824836	5.0180078	2.782483581	5.018007793
X Variable 1	-0.12127967	0.0211202	-5.742	5.09214E-05	-0.166578	-0.0759813	-0.16657804	-0.07598131

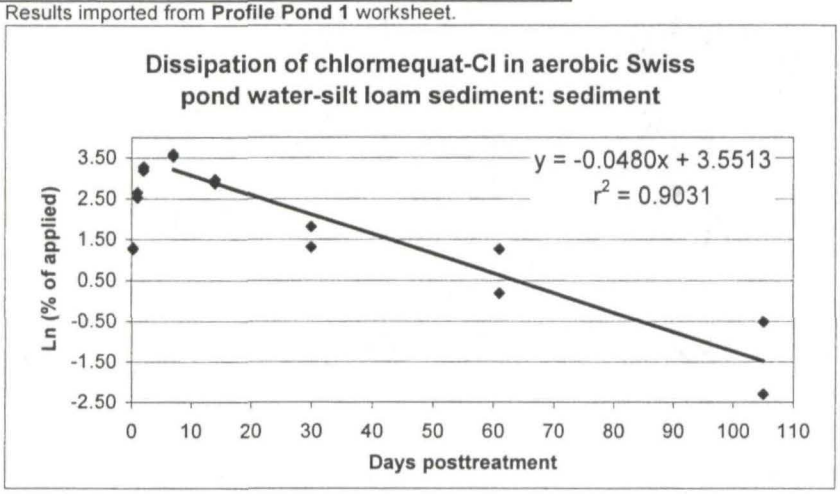
Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Weiherhof-Tal pond water-silt loam sediment.
Half-life determination for sediment.

Half-life (days) 14.5 (7- to 105-day data)

	Chlormequat-chloride	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	0.0	#NUM!
0	0.0	#NUM!
0.25	3.6	1.280933845
0.25	3.5	1.252762968
1	12.5	2.525728644
1	14.1	2.646174797
2	26.3	3.269568939
2	24.2	3.186352633
7	36.2	3.589059119
7	34.3	3.535145354
14	17.8	2.879198457
14	19.3	2.960105096
30	3.7	1.30833282
30	6.1	1.808288771
61	1.2	0.182321557
61	3.5	1.252762968
105	0.6	-0.510825624
105	0.1	-2.302585093

Results imported from **Profile Pond 1** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.95031253
R Square	0.903093904
Adjusted R Square	0.890980642
Standard Error	0.631897782
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	29.7690833	29.769	74.55414592	2.511E-05
Residual	8	3.194358455	0.3993		
Total	9	32.96344175			

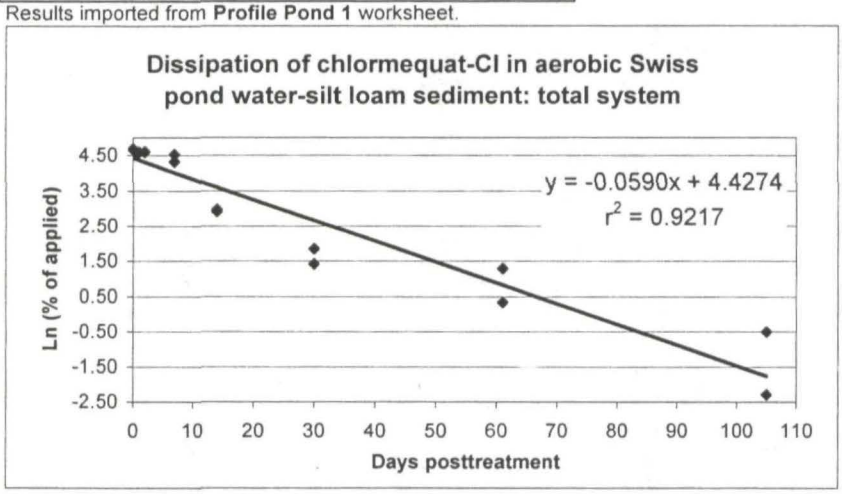
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.551304304	0.313085484	11.343	3.28897E-06	2.8293274	4.2732812	2.82932742	4.273281191
X Variable 1	-0.047952165	0.005553571	-8.634	2.51092E-05	-0.060759	-0.0351456	-0.06075873	-0.0351456

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Weiherhof-Tal pond water-silt loam sediment.
Half-life determination for total system.
Half-life (days) 11.8 (0- to 105-day data)

	Chlormequat-chloride	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	108.1	4.683056725
0	106.1	4.664382046
0.25	101.4	4.619073091
0.25	101.7	4.622027303
1	98.8	4.593097605
1	96.6	4.570578741
2	99.7	4.602165677
2	97.8	4.582924577
7	91.5	4.516338972
7	74.9	4.316153891
14	18.4	2.912350665
14	19.5	2.970414466
30	4.1	1.410986974
30	6.3	1.840549633
61	1.4	0.336472237
61	3.6	1.280933845
105	0.6	-0.510825624
105	0.1	-2.302585093

Results imported from **Profile Pond 1** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.960068423
R Square	0.921731378
Adjusted R Square	0.916839589
Standard Error	0.622949168
Observations	18

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	73.12096	73.121	188.4241934	2.867E-10
Residual	16	6.209050648	0.3881		
Total	17	79.33001065			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.427425086	0.180609792	24.514	4.06695E-14	4.0445495	4.8103007	4.04454952	4.810300654
X Variable 1	-0.058991046	0.004297519	-13.73	2.86728E-10	-0.068101	-0.0498807	-0.06810138	-0.04988072

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Nonlinear half-lives (exponential decay/single, 2 parameter)

Swiss river water-sandy loam sediment.

Phase	water	sediment	system
Half-life (days)	2.6	6.7	4.9
R squared	0.9765	0.8203	0.9803

Swiss pond water-silt loam sediment.

Phase	water	sediment	system
Half-life (days)	4.6	7.9	8.7
R squared	0.9733	0.9898	0.9532

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Determination of means/standard deviations of treated system parameters (pH, O_2 and redox potentials).

Rhine river water-sandy loam sediment.

Day	Water layer pH	Water layer O_2 (mg/L)	Water layer Redox (mV)	Sediment Redox (mV)
0	8.10	6.8	161	-140
	8.28	7.3	161	-122
0.25	8.09	4.5	195	-74
	8.09	3.5	197	-150
1	8.26	5.9	209	-100
	8.46	7.3	201	-80
2	8.07	5.8	204	-111
	8.20	7.3	199	-101
7	8.09	6.9	203	-135
	8.13	7.2	200	-94
14	8.19	6.3	151	-130
	8.24	5.5	153	-129
30	8.04	6.9	180	-144
	8.14	7.8	176	-140
61	8.15	6.5	62	-158
	8.31	7.3	54	-162
105	8.51	7.2	180	-184
	8.45	7.6	181	-211
Mean	8.21	6.5	170	-131
std.dev.	0.14	1.1	44	34
n =	18	18	18	18

Weiherhof-Tal pond water-silt loam sediment.

Day	Water layer pH	Water layer O_2 (mg/L)	Water layer Redox (mV)	Sediment Redox (mV)
0	7.94	5.9	162	-99
	8.29	5.7	163	-95
0.25	8.05	5.3	201	-101
	8.14	4.6	189	-111
1	8.14	7.0	210	-111
	8.15	6.9	210	-115
2	8.07	7.6	207	-87
	8.13	7.5	202	-102
7	8.09	7.5	171	-107
	8.14	8.3	202	-106
14	8.01	6.8	160	-127
	8.07	7.5	158	-83
30	7.88	8.0	193	-104
	7.96	7.6	190	-109
61	7.46	5.3	51	-107
	7.89	7.0	42	-85
105	8.36	8.2	139	-136
	8.13	6.7	184	-120
Mean	8.05	6.9	169	-106
std.dev.	0.19	1.0	48	13
n =	18	18	18	18

Both systems.

Mean	8.13	6.7	169	-119
std.dev.	0.18	1.1	46	29
n =	36	36	36	36

Results from Tables 6-7, pp. 56-59 of the study report; treated systems only.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.
Rhine river water-sandy loam sediment.

				Sediment														
	Water			Extracts			Nonextractable			CO_2			Material Balance			Study Reported Material Balance		
Day	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	105.4						2.6						108.0			107.9		
	105.7	105.6	0.1		#####	#####	1.3	2.0	0.7		#####	#####	107.0	107.5	0.5	107.0	107.5	0.5
0.25	93.1			6.9			6.3						106.3			106.3		
	84.3	88.7	4.4	11.2	9.1	2.1	9.2	7.8	1.5		#####	#####	104.7	105.5	0.8	104.7	105.5	0.8
1	72.8			23.0			8.8			0.1			104.7			104.6		
	73.4	73.1	0.3	22.5	22.8	0.3	6.5	7.7	1.2	0.1	0.1	0.0	102.5	103.6	1.1	102.4	103.5	1.1
2	59.7			34.4			10.8			0.1			105.0			105.0		
	63.9	61.8	2.1	30.3	32.4	2.0	10.3	10.6	0.3	0.3	0.2	0.1	104.8	104.9	0.1	104.7	104.9	0.1
7	3.0			40.1			30.9			26.9			100.9			100.9		
	25.6	14.3	11.3	15.7	27.9	12.2	37.5	34.2	3.3	10.8	18.9	8.0	89.6	95.3	5.7	89.7	95.3	5.6
14	2.8			19.6			36.6			19.7			78.7			78.6		
	2.2	2.5	0.3	9.5	14.6	5.1	42.6	39.6	3.0	35.2	27.5	7.7	89.5	84.1	5.4	89.5	84.1	5.5
30	2.4			5.8			37.5			43.8			89.5			89.6		
	2.0	2.2	0.2	2.9	4.4	1.5	49.0	43.3	5.8	49.8	46.8	3.0	103.7	96.6	7.1	103.7	96.7	7.0
61	1.4			2.0			35.2			57.9			96.5			96.6		
	1.3	1.4	0.0	1.8	1.9	0.1	30.7	33.0	2.3	65.5	61.7	3.8	99.3	97.9	1.4	99.3	98.0	1.4
105	0.5			1.2			27.7			64.1			93.5			93.5		
	0.4	0.5	0.1	0.9	1.1	0.2	26.2	27.0	0.8	69.9	67.0	2.9	97.4	95.5	1.9	97.4	95.5	1.9
													Overall	99.0	7.8		99.0	7.8

Results from Table 9, p. 61 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Both systems:				
Mean	s.d.	n	Max.	Min.
98.7	9.4	36	76.2	109.5

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.

Rhine river water-sandy loam sediment.
Total [^{14}C]residues in sediment.

	Sediment				
	Ext.	Nonext.	Total in Sediment		
Day	% AR	% AR	% AR	Mean	s.d.
0	0.0	2.6	2.6		
	0.0	1.3	1.3	2.0	0.7
0.25	6.9	6.3	13.2		
	11.2	9.2	20.4	16.8	3.6
1	23.0	8.8	31.8		
	22.5	6.5	29.0	30.4	1.4
2	34.4	10.8	45.2		
	30.3	10.3	40.6	42.9	2.3
7	40.1	30.9	71.0		
	15.7	37.5	53.2	62.1	8.9
14	19.6	36.6	56.2		
	9.5	42.6	52.1	54.2	2.0
30	5.8	37.5	43.3		
	2.9	49.0	51.9	47.6	4.3
61	2.0	35.2	37.2		
	1.8	30.7	32.5	34.9	2.4
105	1.2	27.7	28.9		
	0.9	26.2	27.1	28.0	0.9

[14C]Residue water phase:sediment ratios.

	Water	Sed.	Ratio	Ratio	W:S ratio		S:W ratio	
Day	% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
0	105.4	2.6	41	0				
	105.7	1.3	81	0	61	20	0	0
0.25	93.1	13.2	7	0				
	84.3	20.4	4	0	6	1	0	0
1	72.8	31.8	2	0				
	73.4	29.0	3	0	2	0	0	0
2	59.7	45.2	1	1				
	63.9	40.6	2	1	1	0	1	0
7	3.0	71.0	0	24				
	25.6	53.2	0	2	0	0	13	11
14	2.8	56.2	0	20				
	2.2	52.1	0	24	0	0	22	2
30	2.4	43.3	0	18				
	2.0	51.9	0	26	0	0	22	4
61	1.4	37.2	0	27				
	1.3	32.5	0	25	0	0	26	1
105	0.5	28.9	0	58				
	0.4	27.1	0	68	0	0	63	5

Results imported from **Mat bal River** worksheet.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.
Weiherhof-Tal pond water-silt loam sediment.

	Water			Sediment						CO_2			Material Balance			Study Reported Material Balance		
				Extracts			Nonextractable											
Day	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	108.1						1.4						109.5			109.5		
	106.1	107.1	1.0		#####	#####	1.0	1.2	0.2		#####	#####	107.1	108.3	1.2	107.1	108.3	1.2
0.25	97.9			3.6			5.9						107.4			107.3		
	98.2	98.1	0.1	3.5	3.6	0.1	5.9	5.9	0.0		#####	#####	107.6	107.5	0.1	107.6	107.5	0.1
1	86.3			13.0			8.5			0.1			107.9			107.8		
	82.5	84.4	1.9	14.1	13.6	0.5	9.6	9.1	0.5		0.1	0.0	106.2	107.1	0.9	106.2	107.0	0.8
2	74.1			26.3			5.7			0.1			106.2			106.2		
	76.4	75.3	1.2	24.2	25.3	1.0	5.5	5.6	0.1	0.1	0.1	0.0	106.2	106.2	0.0	106.2	106.2	0.0
7	57.0			38.8			9.3			0.5			105.6			105.5		
	43.1	50.1	7.0	36.7	37.8	1.0	17.2	13.3	4.0	3.2	1.9	1.4	100.2	102.9	2.7	100.1	102.8	2.7
14	2.4			19.4			37.3			26.8			85.9			85.9		
	2.4	2.4	0.0	21.0	20.2	0.8	36.8	37.1	0.3	25.1	26.0	0.8	85.3	85.6	0.3	85.3	85.6	0.3
30	1.4			12.8			59.2			35.0			108.4			108.4		
	0.9	1.2	0.3	8.1	10.5	2.4	46.5	52.9	6.4	32.3	33.7	1.4	87.8	98.1	10.3	87.9	98.2	10.3
61	0.5			2.6			34.7			50.6			88.4			88.3		
	0.5	0.5	0.0	4.8	3.7	1.1	35.9	35.3	0.6	34.9	42.8	7.9	76.1	82.3	6.2	76.2	82.3	6.1
105	0.1			2.0			31.3			54.1			87.5			87.5		
	0.1	0.1	0.0	1.1	1.6	0.5	28.6	30.0	1.3	57.1	55.6	1.5	86.9	87.2	0.3	87.0	87.3	0.3
												Overall		98.3	10.8		98.3	10.7

Results from Table 11, p. 63 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.

Weiherhof-Tal pond water-silt loam sediment.
Total [^{14}C]residues in sediment.

Day	Sediment				
	Ext.	Nonext.	Total in Sediment		
	% AR	% AR	% AR	Mean	s.d.
0	0.0	1.4	1.4		
	0.0	1.0	1.0	1.2	0.2
0.25	3.6	5.9	9.5		
	3.5	5.9	9.4	9.5	0.0
1	13.0	8.5	21.5		
	14.1	9.6	23.7	22.6	1.1
2	26.3	5.7	32.0		
	24.2	5.5	29.7	30.9	1.1
7	38.8	9.3	48.1		
	36.7	17.2	53.9	51.0	2.9
14	19.4	37.3	56.7		
	21.0	36.8	57.8	57.3	0.5
30	12.8	59.2	72.0		
	8.1	46.5	54.6	63.3	8.7
61	2.6	34.7	37.3		
	4.8	35.9	40.7	39.0	1.7
105	2.0	31.3	33.3		
	1.1	28.6	29.7	31.5	1.8

[14C]Residue water phase:sediment ratios.

Day	Water	Sed.	Ratio	Ratio	W:S ratio		S:W ratio	
	% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
0	108.1	1.4	77	0				
	106.1	1.0	106	0	92	14	0	0
0.25	97.9	9.5	10	0				
	98.2	9.4	10	0	10	0	0	0
1	86.3	21.5	4	0				
	82.5	23.7	3	0	4	0	0	0
2	74.1	32.0	2	0				
	76.4	29.7	3	0	2	0	0	0
7	57.0	48.1	1	1				
	43.1	53.9	1	1	1	0	1	0
14	2.4	56.7	0	24				
	2.4	57.8	0	24	0	0	24	0
30	1.4	72.0	0	51				
	0.9	54.6	0	61	0	0	56	5
61	0.5	37.3	0	75				
	0.5	40.7	0	81	0	0	78	3
105	0.1	33.3	0	333				
	0.1	29.7	0	297	0	0	315	18

Results imported from **Mat bal Pond** worksheet.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Confirmation/determination of means/std.dev. for [^{14}C]chlormequat-chloride and its transformation products.
Rhine river water-sandy loam sediment.

	Chlormequat-chloride									RW1/RS1 (Rf = 0.97 in SS3, 0.34/0.50 in SS4)									RW2/RS2 (Rf = 0.61 in SS3, 0.27/0.34 in SS4)								
	Water			Sediment			Total system			Water			Sediment			Total system			Water			Sediment			Total system		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	105.4						105.4									0.0									0.0		
	105.7	105.6	0.1		####	####	105.7	105.6	0.1		####	####		####	####	0.0	0.0	0.0		####	####		####	####	0.0	0.0	0.0
0.25	91.6			6.9			98.4									0.0									0.0		
	79.2	85.4	6.2	11.2	9.1	2.1	90.3	94.4	4.1		####	####		####	####	0.0	0.0	0.0		####	####		####	####	0.0	0.0	0.0
1	72.8			23.0			95.8									0.0									0.0		
	73.4	73.1	0.3	22.5	22.8	0.3	95.9	95.9	0.1		####	####		####	####	0.0	0.0	0.0		####	####		####	####	0.0	0.0	0.0
2	59.7			34.4			94.1									0.0									0.0		
	63.9	61.8	2.1	30.3	32.4	2.0	94.1	94.1	0.0		####	####		####	####	0.0	0.0	0.0		####	####		####	####	0.0	0.0	0.0
7	2.9			37.4			40.3									0.0									0.0		
	25.6	14.3	11.4	11.8	24.6	12.8	37.4	38.9	1.4		####	####		####	####	0.0	0.0	0.0		####	####		####	####	0.0	0.0	0.0
14	0.5			8.5			9.0									0.0									0.0		
	0.4	0.5	0.1	4.0	6.3	2.3	4.4	6.7	2.3		####	####		####	####	0.0	0.0	0.0		####	####		####	####	0.0	0.0	0.0
30	0.4			1.3			1.7			0.2						0.2			0.2						0.2		
	0.3	0.4	0.1	1.7	1.5	0.2	2.0	1.9	0.2	0.2	0.2	0.0		####	####	0.2	0.2	0.0	0.2	0.2	0.0	<0.1	####	####	####	####	####
61	0.3			0.5			0.7									0.0									0.0		
		0.3	0.0	0.4	0.5	0.1	0.4	0.6	0.2	0.1	0.1	0.0	<0.1	####	####	####	####	####		####	####		####	####	0.0	0.0	0.0
105				0.1			0.1						<0.1			####									0.0		
		####	####	0.2	0.2	0.1	0.2	0.2	0.1		####	####		####	####	0.0	####	####		####	####		####	####	0.0	0.0	0.0

Results from Tables 13-14, pp. 65-66; Table 16, p. 68 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Confirmation/determination of means/std.dev. for [^{14}C]chlormequat-chloride and its transformation products (continued).
Rhine river water-sandy loam sediment.

	RW3/RS3 (Rf = 0.44 in SS3, 0.13 in SS4)									RW4/RS4 (Rf = 0.01-0.02 in SS3 and SS4)								
	Water			Sediment			Total system			Water			Sediment			Total system		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		####	####		####	####	0.0 0.0	0.0	0.0		####	####		####	####	0.0 0.0	0.0	0.0
0.25	3.4	3.4	0.0		####	####	0.0 3.4	1.7	1.7	1.6 1.8	1.7	0.1		####	####	1.6 1.8	1.7	0.1
1		####	####		####	####	0.0 0.0	0.0	0.0		####	####		####	####	0.0 0.0	0.0	0.0
2		####	####		####	####	0.0 0.0	0.0	0.0		####	####		####	####	0.0 0.0	0.0	0.0
7		####	####		####	####	0.0 0.0	0.0	0.0	0.1	0.1	0.0	2.7 3.9	3.3	0.6	2.8 3.9	3.4	0.6
14		####	####		####	####	0.0 0.0	0.0	0.0	2.3 1.8	2.1	0.3	11.1 5.5	8.3	2.8	13.4 7.3	10.4	3.1
30	0.3 0.2	0.3	0.1	1.7 0.8	1.3	0.5	2.0 1.0	1.5	0.5	1.4 1.1	1.3	0.2	2.7 0.3	1.5	1.2	4.1 1.4	2.8	1.4
61		####	####	<0.1	####	####	0.0 ####	####	####	1.2 1.3	1.3	0.0	1.6 1.4	1.5	0.1	2.8 2.7	2.8	0.0
105		####	####	0.2 0.2	0.2	0.0	0.2 0.2	0.2	0.0	0.6 0.4	0.5	0.1	0.8 0.6	0.7	0.1	1.4 1.0	1.2	0.2

Results from Table 14, p. 66; Table 16, p. 68 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Confirmation/determination of means/std.dev. for [^{14}C]chlormequat-chloride and its transformation products.
Weiherhof-Tal pond water-silt loam sediment.

	Chlormequat-chloride									PW1/PS1 (Rf = 0.98 in SS3, 0.3/0.5 in SS4)								
	Water			Sediment			Total system			Water			Sediment			Total system		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	108.1						108.1									0.0		
	106.1	107.1	1.0		####	####	106.1	107.1	1.0		####	####		####	####	0.0	0.0	0.0
0.25	97.9			3.6			101.4									0.0		
	98.2	98.1	0.1	3.5	3.6	0.1	101.7	101.6	0.1		####	####		####	####	0.0	0.0	0.0
1	86.3			12.5			98.8									0.0		
	82.5	84.4	1.9	14.1	13.3	0.8	96.6	97.7	1.1		####	####		####	####	0.0	0.0	0.0
2	73.4			26.3			99.7									0.0		
	73.6	73.5	0.1	24.2	25.3	1.0	97.8	98.8	1.0		####	####		####	####	0.0	0.0	0.0
7	55.3			36.2			91.5									0.0		
	40.6	48.0	7.3	34.3	35.3	1.0	74.9	83.2	8.3		####	####		####	####	0.0	0.0	0.0
14	0.6			17.8			18.4									0.0		
	0.2	0.4	0.2	19.3	18.6	0.8	19.5	19.0	0.5		####	####		####	####	0.0	0.0	0.0
30	0.4			3.7			4.1			0.1						0.1		
	0.1	0.3	0.2	6.1	4.9	1.2	6.3	5.2	1.1	<0.1	0.1	0.0		####	####	####	####	####
61	0.2			1.2			1.4						0.1			0.1		
	0.1	0.2	0.1	3.5	2.4	1.2	3.6	2.5	1.1		####	####		0.1	0.0	0.0	0.1	0.1
105				0.6			0.6									0.0		
		####	####	0.1	0.4	0.3	0.1	0.4	0.3		####	####		####	####	0.0	0.0	0.0

Results from Tables 18-19, pp. 70-71; Table 21, p. 73 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

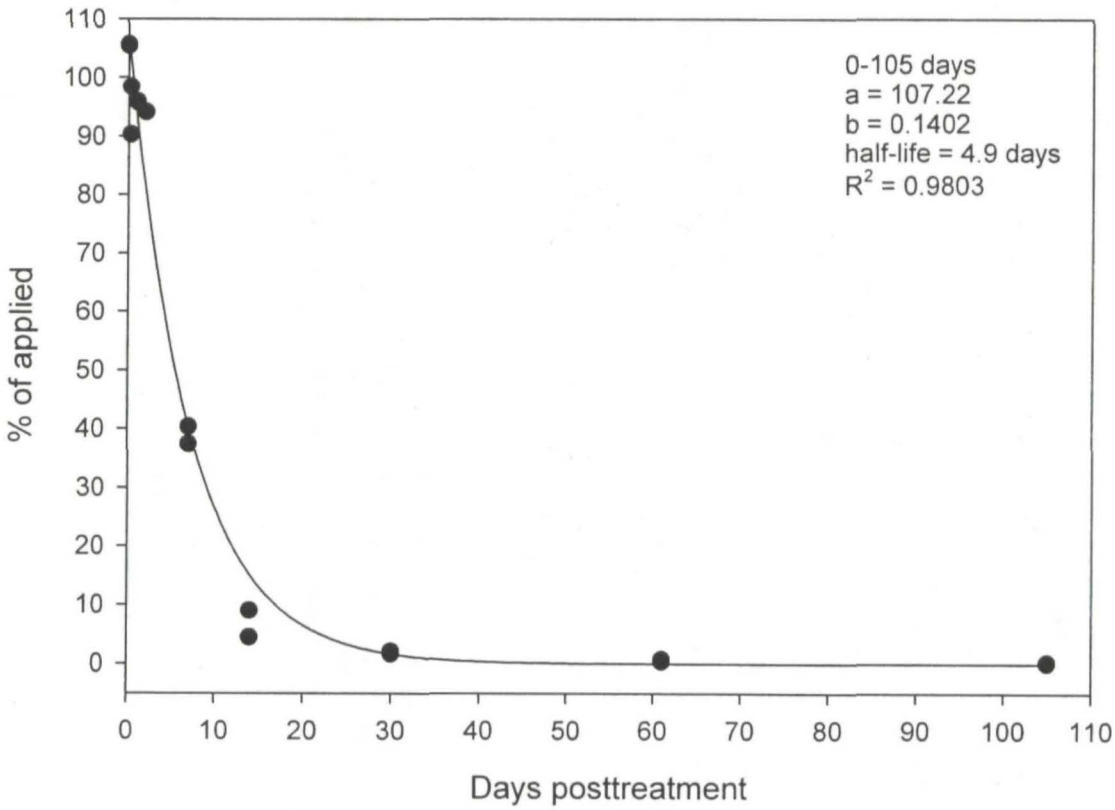
Chemical: Chlormequat-chloride
PC: 018101
MRID: 46715227
Guideline: 162-4

Aerobic aquatic metabolism of [^{14}C]chlormequat-chloride in two Swiss water-sediment systems.
Confirmation/determination of means/std.dev. for [^{14}C]chlormequat-chloride and its transformation products (continued).
Weiherhof-Tal pond water-silt loam sediment.

	PW2/PS2 (Rf = 0.49 in SS3, 0.18/0.13 in SS4)									PW3/PS3 (Rf = 0.01-0.02 in SS3, SS4)								
	Water			Sediment			Total system			Water			Sediment			Total system		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		####	####		####	####	0.0 0.0	0.0	0.0		####	####		####	####	0.0 0.0	0.0	0.0
0.25		####	####		####	####	0.0 0.0	0.0	0.0		####	####		####	####	0.0 0.0	0.0	0.0
1		####	####		####	####	0.0 0.0	0.0	0.0		####	####		####	####	0.0 0.0	0.0	0.0
2		####	####		####	####	0.0 0.0	0.0	0.0	0.7 2.8	1.8	1.1		####	####	0.7 2.8	1.8	1.1
7		####	####		####	####	0.0 0.0	0.0	0.0	1.7 2.5	2.1	0.4	2.3	2.3	0.0	1.7 4.8	3.3	1.6
14	0.5	0.5	0.0		####	####	0.5	0.5	0.0	1.8 1.6	1.7	0.1	1.6 1.7	1.7	0.1	3.4 3.3	3.4	0.1
30	0.3 0.1	0.2	0.1	5.2 1.1	3.2	2.1	5.5 1.2	3.4	2.2	0.6 0.6	0.6	0.0	4.0 0.9	2.5	1.6	4.6 1.5	3.1	1.6
61	0.1 0.1	0.1	0.0	0.7 0.9	0.8	0.1	0.8 1.0	0.9	0.1	0.2 0.2	0.2	0.0	0.6 0.5	0.6	0.0	0.8 0.7	0.8	0.1
105		####	####	0.7 0.1	0.4	0.3	0.7 0.1	0.4	0.3	0.1 0.1	0.1	0.0	0.6 0.9	0.8	0.2	0.7 1.0	0.9	0.2

Results from Table 19, p. 71; Table 21, p. 73 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Dissipation of chlormequat-Cl in aerobic Swiss river water-sandy loam sediment: total system, nonlinear regression (MRID 46715227)



Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
Swiss Rhine river water-sandy loam sediment
Total system
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 107.221}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.140203}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.99010342 Rsqr = 0.98030479 Adj Rsqr = 0.97907383

Standard Error of Estimate = 6.7223

	Coefficient	Std. Error	t	P
a	107.2208	2.9481	36.3698	<0.0001
b	0.1402	0.0135	10.3543	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	35987.8737	35987.8737	796.3801	<0.0001
Residual	16	723.0291	45.1893		
Total	17	36710.9028	2159.4649		

PRESS = 973.3985

Durbin-Watson Statistic = 1.0544

Normality Test: K-S Statistic = 0.2362 Significance Level = 0.2328

Constant Variance Test: Failed (P = 0.0150)

Power of performed test with alpha = 0.0500: 1.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Rhine river water-sandy loam sediment
Total system

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	107.2208	-1.8208	-0.2709	-0.3014	-0.2927
2	107.2208	-1.5208	-0.2262	-0.2517	-0.2442
3	103.5278	-5.1278	-0.7628	-0.8325	-0.8241
4	103.5278	-13.2278	-1.9677	-2.1475	-2.4647
5	93.1944	2.6056	0.3876	0.4110	0.4000
6	93.1944	2.7056	0.4025	0.4267	0.4156
7	81.0028	13.0972	1.9483	2.0657	2.3356
8	81.0028	13.0972	1.9483	2.0657	2.3356
9	40.1840	0.1160	0.0173	0.0200	0.0194
10	40.1840	-2.7840	-0.4141	-0.4807	-0.4688
11	15.0600	-6.0600	-0.9015	-0.9835	-0.9824
12	15.0600	-10.6600	-1.5858	-1.7300	-1.8578
13	1.5981	0.1019	0.0152	0.0152	0.0147
14	1.5981	0.4019	0.0598	0.0601	0.0582
15	0.0207	0.6793	0.1011	0.1011	0.0979
16	0.0207	0.3793	0.0564	0.0564	0.0546
17	0.0000	0.1000	0.0149	0.0149	0.0144
18	0.0000	0.2000	0.0297	0.0297	0.0288

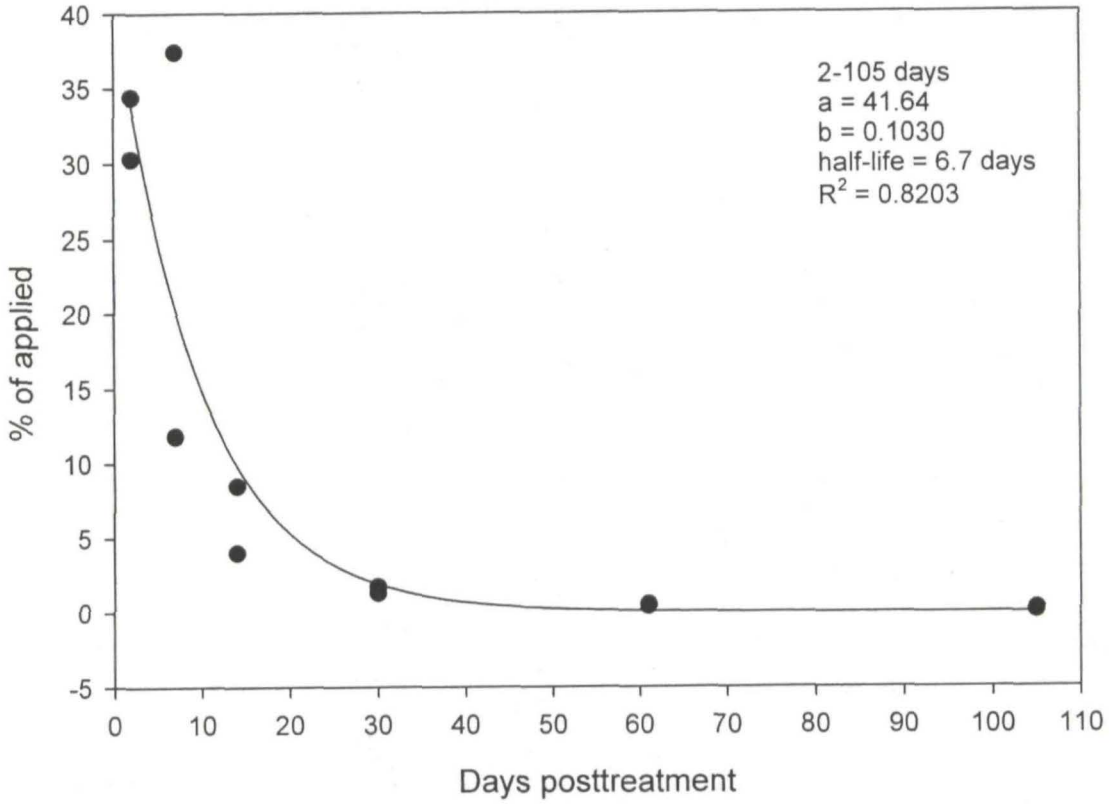
Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.0108	0.1923	-0.1428
2	0.0075	0.1923	-0.1192
3	0.0662	0.1604	-0.3602
4	0.4406	0.1604	-1.0773
5	0.0105	0.1105	0.1410
6	0.0113	0.1105	0.1465
7	0.2648	0.1104	0.8229
8	0.2648	0.1104	0.8229
9	0.0001	0.2577	0.0114
10	0.0401	0.2577	-0.2762
11	0.0919	0.1598	-0.4283
12	0.2845	0.1598	-0.8100
13	0.0000	0.0089	0.0014
14	0.0000	0.0089	0.0055
15	0.0000	0.0000	0.0002
16	0.0000	0.0000	0.0001
17	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Rhine river water-sandy loam sediment
Total system
95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	107.2208	100.9712	113.4705	91.6600	122.7816
2	107.2208	100.9712	113.4705	91.6600	122.7816
3	103.5278	97.8200	109.2355	88.1766	118.8790
4	103.5278	97.8200	109.2355	88.1766	118.8790
5	93.1944	88.4576	97.9312	78.1771	108.2116
6	93.1944	88.4576	97.9312	78.1771	108.2116
7	81.0028	76.2676	85.7381	65.9861	96.0196
8	81.0028	76.2676	85.7381	65.9861	96.0196
9	40.1840	32.9498	47.4181	24.2023	56.1656
10	40.1840	32.9498	47.4181	24.2023	56.1656
11	15.0600	9.3642	20.7559	-0.2867	30.4068
12	15.0600	9.3642	20.7559	-0.2867	30.4068
13	1.5981	0.2535	2.9426	-12.7159	15.9120
14	1.5981	0.2535	2.9426	-12.7159	15.9120
15	0.0207	-0.0156	0.0570	-14.2300	14.2714
16	0.0207	-0.0156	0.0570	-14.2300	14.2714
17	0.0000	-0.0001	0.0002	-14.2506	14.2507
18	0.0000	-0.0001	0.0002	-14.2506	14.2507

Dissipation of chlormequat-Cl in aerobic Swiss river water-sandy loam sediment: sediment, nonlinear regression (MRID 46715227)



Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
Swiss Rhine river water-sandy loam sediment
Sediment
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 41.6356}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.102992}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.90569229 Rsqr = 0.82027852 Adj Rsqr = 0.80230637

Standard Error of Estimate = 6.4452

	Coefficient	Std. Error	t	P
a	41.6356	7.0984	5.8655	0.0002
b	0.1030	0.0322	3.2025	0.0095

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	1895.9726	1895.9726	45.6417	<0.0001
Residual	10	415.4040	41.5404		
Total	11	2311.3767	210.1252		

PRESS = 706.7254

Durbin-Watson Statistic = 2.8914

Normality Test: K-S Statistic = 0.3833 Significance Level = 0.0429

Constant Variance Test: Failed (P = 0.0040)

Power of performed test with alpha = 0.0500: 0.9946

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Rhine river water-sandy loam sediment
Sediment

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	33.8849	0.5151	0.0799	0.1087	0.1031
2	33.8849	-3.5849	-0.5562	-0.7563	-0.7390
3	20.2470	17.1530	2.6614	3.0051	9.1555
4	20.2470	-8.4470	-1.3106	-1.4799	-1.5886
5	9.8460	-1.3460	-0.2088	-0.2438	-0.2320
6	9.8460	-5.8460	-0.9070	-1.0589	-1.0661
7	1.8949	-0.5949	-0.0923	-0.0951	-0.0903
8	1.8949	-0.1949	-0.0302	-0.0312	-0.0296
9	0.0778	0.4222	0.0655	0.0655	0.0622
10	0.0778	0.3222	0.0500	0.0500	0.0474
11	0.0008	0.0992	0.0154	0.0154	0.0146
12	0.0008	0.1992	0.0309	0.0309	0.0293

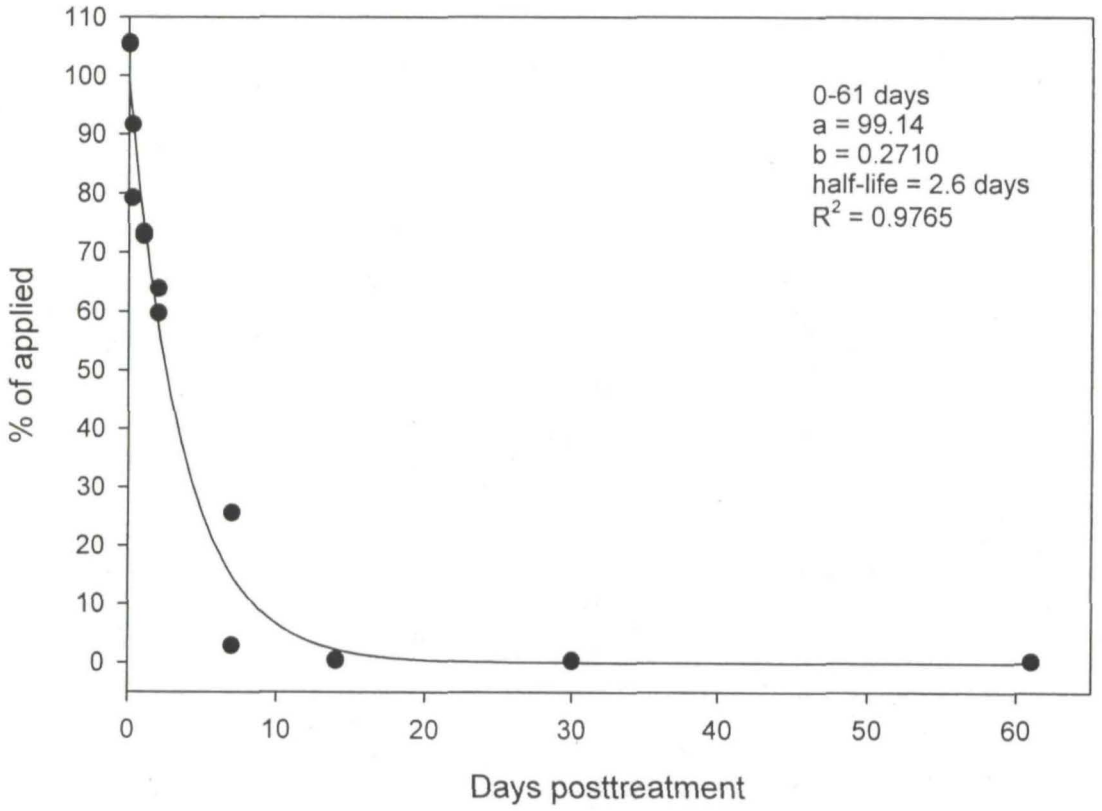
Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.0050	0.4592	0.0950
2	0.2428	0.4592	-0.6809
3	1.2416	0.2157	4.8009
4	0.3011	0.2157	-0.8330
5	0.0108	0.2663	-0.1397
6	0.2034	0.2663	-0.6422
7	0.0003	0.0585	-0.0225
8	0.0000	0.0585	-0.0074
9	0.0000	0.0004	0.0013
10	0.0000	0.0004	0.0010
11	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	33.8849	24.1538	43.6161	16.5377	51.2322
2	33.8849	24.1538	43.6161	16.5377	51.2322
3	20.2470	13.5779	26.9162	4.4132	36.0808
4	20.2470	13.5779	26.9162	4.4132	36.0808
5	9.8460	2.4358	17.2561	-6.3139	26.0059
6	9.8460	2.4358	17.2561	-6.3139	26.0059
7	1.8949	-1.5775	5.3674	-12.8797	16.6696
8	1.8949	-1.5775	5.3674	-12.8797	16.6696
9	0.0778	-0.2230	0.3786	-14.2861	14.4417
10	0.0778	-0.2230	0.3786	-14.2861	14.4417
11	0.0008	-0.0046	0.0063	-14.3599	14.3616
12	0.0008	-0.0046	0.0063	-14.3599	14.3616

Dissipation of chlormequat-Cl in aerobic Swiss river water-sandy loam sediment: water layer, nonlinear regression (MRID 46715227)



Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
Swiss Rhine river water-sandy loam sediment
Water layer
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 99.1412}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.271001}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.98819510 Rsqr = 0.97652955 Adj Rsqr = 0.97472413

Standard Error of Estimate = 6.7084

	Coefficient	Std. Error	t	P
a	99.1412	3.3779	29.3500	<0.0001
b	0.2710	0.0320	8.4656	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	24341.6682	24341.6682	540.8880	<0.0001
Residual	13	585.0411	45.0032		
Total	14	24926.7093	1780.4792		

PRESS = 924.3347

Durbin-Watson Statistic = 2.3384

Normality Test: K-S Statistic = 0.1987 Significance Level = 0.5457

Constant Variance Test: Failed (P = 0.0136)

Power of performed test with alpha = 0.0500: 1.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Rhine river water-sandy loam sediment
Water layer

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	99.1412	6.2588	0.9330	1.0799	1.0874
2	99.1412	6.5588	0.9777	1.1316	1.1451
3	92.6469	-1.0469	-0.1561	-0.1720	-0.1654
4	92.6469	-13.4469	-2.0045	-2.2091	-2.6855
5	75.6067	-2.8067	-0.4184	-0.4475	-0.4333
6	75.6067	-2.2067	-0.3289	-0.3518	-0.3397
7	57.6589	2.0411	0.3043	0.3428	0.3308
8	57.6589	6.2411	0.9303	1.0481	1.0524
9	14.8729	-11.9729	-1.7848	-2.0096	-2.3255
10	14.8729	10.7271	1.5990	1.8005	1.9967
11	2.2312	-1.7312	-0.2581	-0.2607	-0.2512
12	2.2312	-1.8312	-0.2730	-0.2758	-0.2658
13	0.0292	0.3708	0.0553	0.0553	0.0531
14	0.0292	0.2708	0.0404	0.0404	0.0388
15	0.0000	0.3000	0.0447	0.0447	0.0430

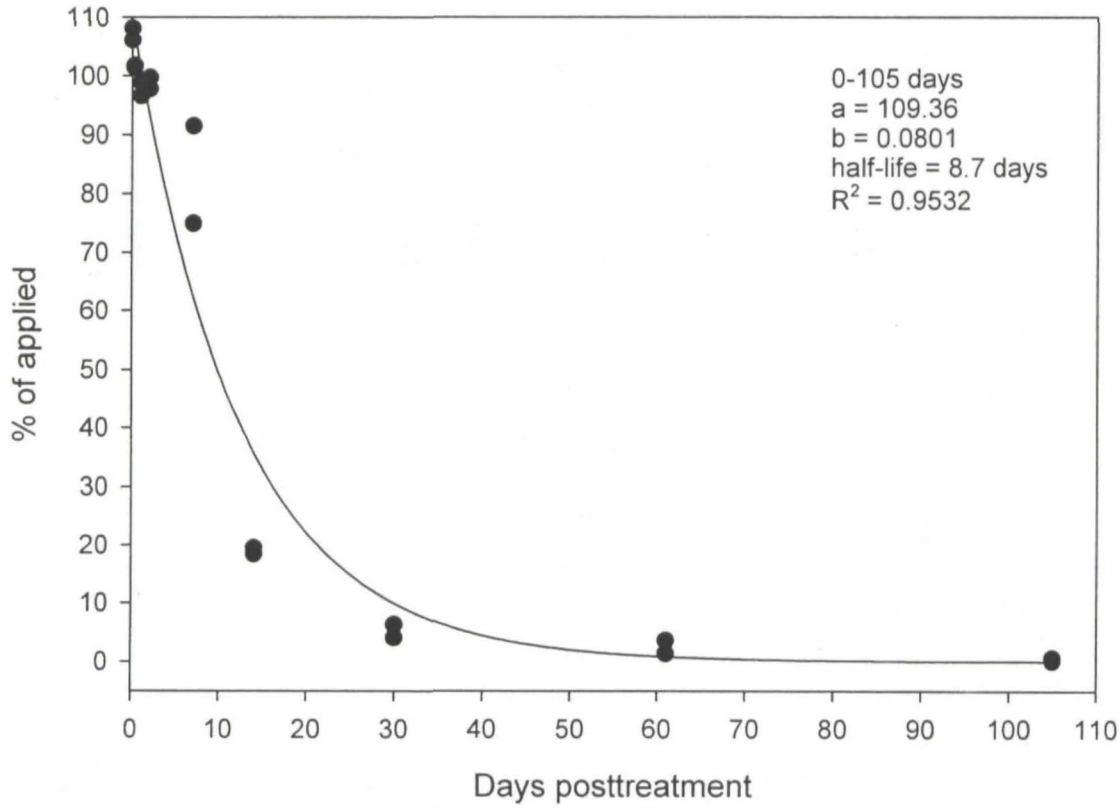
Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.1980	0.2535	0.6337
2	0.2175	0.2535	0.6674
3	0.0032	0.1767	-0.0766
4	0.5236	0.1767	-1.2441
5	0.0144	0.1259	-0.1645
6	0.0089	0.1259	-0.1289
7	0.0158	0.2121	0.1716
8	0.1479	0.2121	0.5461
9	0.5409	0.2113	-1.2035
10	0.4342	0.2113	1.0334
11	0.0007	0.0205	-0.0363
12	0.0008	0.0205	-0.0384
13	0.0000	0.0000	0.0002
14	0.0000	0.0000	0.0002
15	0.0000	0.0000	0.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Rhine river water-sandy loam sediment
Water layer
95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	99.1412	91.8437	106.4387	82.9149	115.3675
2	99.1412	91.8437	106.4387	82.9149	115.3675
3	92.6469	86.5551	98.7387	76.9259	108.3678
4	92.6469	86.5551	98.7387	76.9259	108.3678
5	75.6067	70.4637	80.7496	60.2285	90.9848
6	75.6067	70.4637	80.7496	60.2285	90.9848
7	57.6589	50.9843	64.3334	41.7030	73.6147
8	57.6589	50.9843	64.3334	41.7030	73.6147
9	14.8729	8.2115	21.5343	-1.0774	30.8232
10	14.8729	8.2115	21.5343	-1.0774	30.8232
11	2.2312	0.1580	4.3044	-12.4090	16.8714
12	2.2312	0.1580	4.3044	-12.4090	16.8714
13	0.0292	-0.0301	0.0885	-14.4636	14.5220
14	0.0292	-0.0301	0.0885	-14.4636	14.5220
15	0.0000	-0.0000	0.0000	-14.4927	14.4927

Dissipation of chlormequat-Cl in aerobic Swiss pond water-silt loam sediment: total system, nonlinear regression (MRID 46715227)



Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
Swiss Weiherhof-Tal pond water-silt loam sediment
Total system
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 109.355}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.0800979}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.97630200 Rsqr = 0.95316560 Adj Rsqr = 0.95023845

Standard Error of Estimate = 10.5370

	Coefficient	Std. Error	t	P
a	109.3552	4.2407	25.7871	<0.0001
b	0.0801	0.0111	7.1972	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	36154.4141	36154.4141	325.6292	<0.0001
Residual	16	1776.4703	111.0294		
Total	17	37930.8844	2231.2285		

PRESS = 2654.3815

Durbin-Watson Statistic = 1.1508

Normality Test: K-S Statistic = 0.1997 Significance Level = 0.4259

Constant Variance Test: Passed (P = 0.3924)

Power of performed test with alpha = 0.0500: 1.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Weiherhof-Tal pond water-silt loam sediment
Total system

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	109.3552	-1.2552	-0.1191	-0.1301	-0.1261
2	109.3552	-3.2552	-0.3089	-0.3375	-0.3279
3	107.1872	-5.7872	-0.5492	-0.5943	-0.5819
4	107.1872	-5.4872	-0.5208	-0.5635	-0.5511
5	100.9377	-2.1377	-0.2029	-0.2153	-0.2087
6	100.9377	-4.3377	-0.4117	-0.4368	-0.4255
7	93.1681	6.5319	0.6199	0.6507	0.6385
8	93.1681	4.6319	0.4396	0.4614	0.4498
9	62.4219	29.0781	2.7596	3.0210	4.4627
10	62.4219	12.4781	1.1842	1.2964	1.3268
11	35.6315	-17.2315	-1.6353	-1.8638	-2.0395
12	35.6315	-16.1315	-1.5309	-1.7448	-1.8774
13	9.8914	-5.7914	-0.5496	-0.5760	-0.5636
14	9.8914	-3.5914	-0.3408	-0.3572	-0.3472
15	0.8258	0.5742	0.0545	0.0546	0.0528
16	0.8258	2.7742	0.2633	0.2636	0.2558
17	0.0243	0.5757	0.0546	0.0546	0.0529
18	0.0243	0.0757	0.0072	0.0072	0.0070

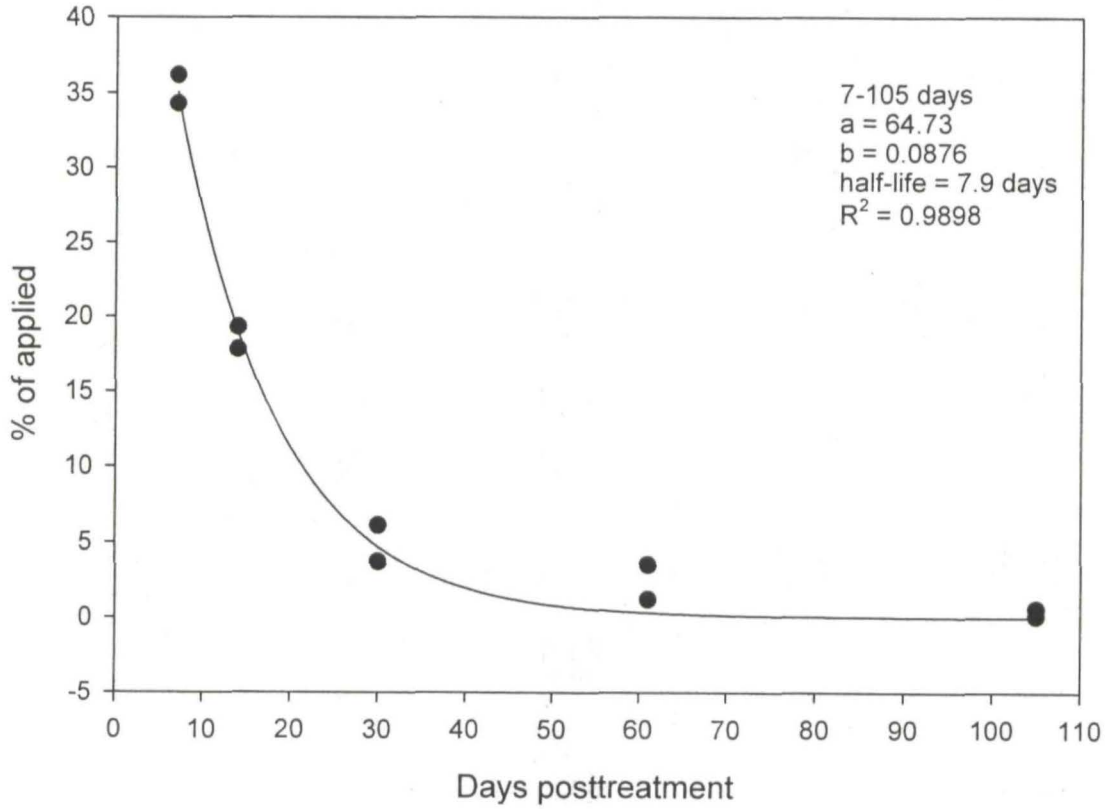
Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.0016	0.1620	-0.0554
2	0.0110	0.1620	-0.1442
3	0.0302	0.1458	-0.2404
4	0.0271	0.1458	-0.2277
5	0.0029	0.1119	-0.0741
6	0.0120	0.1119	-0.1510
7	0.0216	0.0924	0.2037
8	0.0108	0.0924	0.1435
9	0.9053	0.1655	1.9877
10	0.1667	0.1655	0.5910
11	0.5192	0.2301	-1.1151
12	0.4550	0.2301	-1.0265
13	0.0163	0.0895	-0.1767
14	0.0063	0.0895	-0.1089
15	0.0000	0.0027	0.0028
16	0.0001	0.0027	0.0134
17	0.0000	0.0000	0.0001
18	0.0000	0.0000	0.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Weiherhof-Tal pond water-silt loam sediment
Total system
95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	109.3552	100.3653	118.3451	85.2765	133.4339
2	109.3552	100.3653	118.3451	85.2765	133.4339
3	107.1872	98.6566	115.7178	83.2762	131.0982
4	107.1872	98.6566	115.7178	83.2762	131.0982
5	100.9377	93.4666	108.4088	77.3838	124.4915
6	100.9377	93.4666	108.4088	77.3838	124.4915
7	93.1681	86.3780	99.9582	69.8213	116.5149
8	93.1681	86.3780	99.9582	69.8213	116.5149
9	62.4219	53.3333	71.5104	38.3061	86.5376
10	62.4219	53.3333	71.5104	38.3061	86.5376
11	35.6315	24.9155	46.3475	10.8566	60.4064
12	35.6315	24.9155	46.3475	10.8566	60.4064
13	9.8914	3.2092	16.5735	-13.4242	33.2070
14	9.8914	3.2092	16.5735	-13.4242	33.2070
15	0.8258	-0.3423	1.9939	-21.5422	23.1939
16	0.8258	-0.3423	1.9939	-21.5422	23.1939
17	0.0243	-0.0359	0.0846	-22.3133	22.3620
18	0.0243	-0.0359	0.0846	-22.3133	22.3620

Dissipation of chlormequat-Cl in aerobic Swiss pond water-silt loam sediment: sediment, nonlinear regression (MRID 46715227)



Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
Swiss Weiherhof-Tal pond water-silt loam sediment
Sediment
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 64.7284}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.0875924}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.99487987 Rsqr = 0.98978595 Adj Rsqr = 0.98850920

Standard Error of Estimate = 1.4876

	Coefficient	Std. Error	t	P
a	64.7284	4.2684	15.1647	<0.0001
b	0.0876	0.0068	12.8521	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	1715.5326	1715.5326	775.2352	<0.0001
Residual	8	17.7034	2.2129		
Total	9	1733.2360	192.5818		

PRESS = 26.1794

Durbin-Watson Statistic = 1.4703

Normality Test: K-S Statistic = 0.2284 Significance Level = 0.6144

Constant Variance Test: Passed (P = 0.4899)

Power of performed test with alpha = 0.0500: 1.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Weiherhof-Tal pond water-silt loam sediment
Sediment

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	35.0597	1.1403	0.7665	1.0556	1.0643
2	35.0597	-0.7597	-0.5107	-0.7033	-0.6792
3	18.9899	-1.1899	-0.7999	-0.9630	-0.9581
4	18.9899	0.3101	0.2085	0.2510	0.2357
5	4.6759	-0.9759	-0.6560	-0.7389	-0.7160
6	4.6759	1.4241	0.9573	1.0782	1.0909
7	0.3095	0.8905	0.5986	0.6003	0.5746
8	0.3095	3.1905	2.1448	2.1507	3.0976
9	0.0066	0.5934	0.3989	0.3989	0.3769
10	0.0066	0.0934	0.0628	0.0628	0.0588

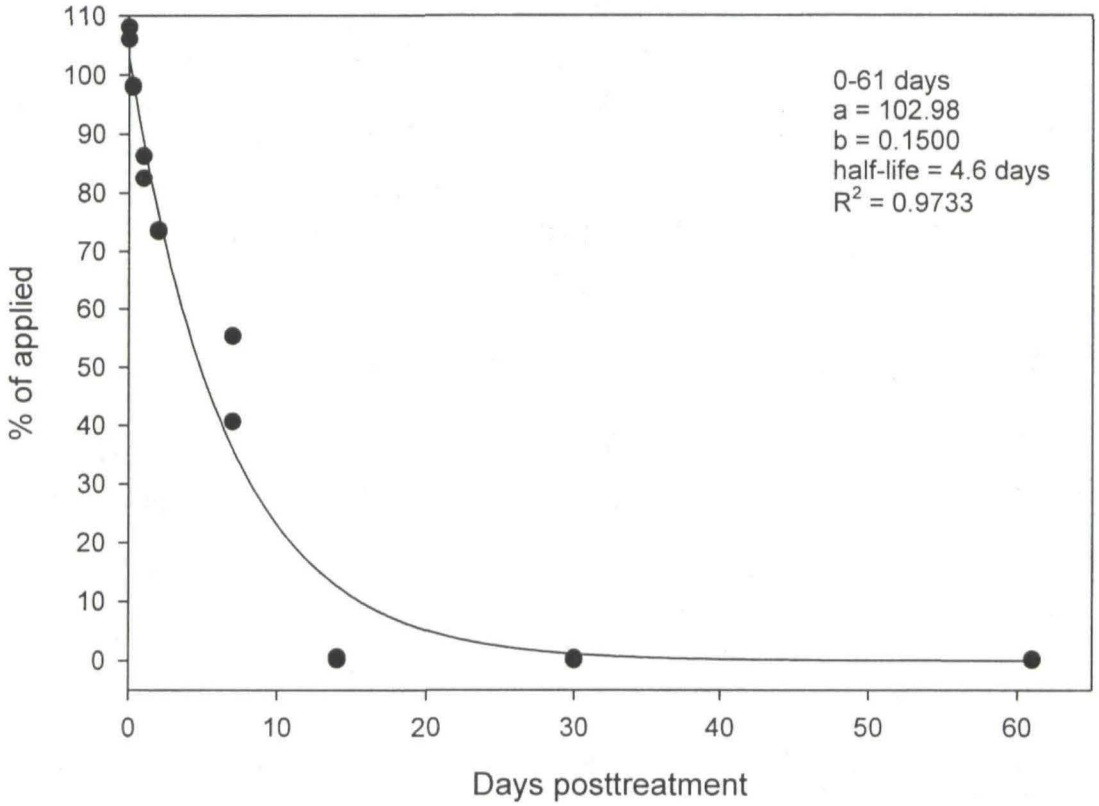
Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.4993	0.4727	1.0076
2	0.2216	0.4727	-0.6430
3	0.2085	0.3102	-0.6425
4	0.0142	0.3102	0.1581
5	0.0733	0.2117	-0.3710
6	0.1560	0.2117	0.5653
7	0.0010	0.0055	0.0427
8	0.0128	0.0055	0.2304
9	0.0000	0.0000	0.0011
10	0.0000	0.0000	0.0002

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	35.0597	32.7013	37.4181	30.8968	39.2226
2	35.0597	32.7013	37.4181	30.8968	39.2226
3	18.9899	17.0794	20.9004	15.0633	22.9164
4	18.9899	17.0794	20.9004	15.0633	22.9164
5	4.6759	3.0978	6.2541	0.8999	8.4519
6	4.6759	3.0978	6.2541	0.8999	8.4519
7	0.3095	0.0550	0.5639	-3.1304	3.7493
8	0.3095	0.0550	0.5639	-3.1304	3.7493
9	0.0066	-0.0034	0.0165	-3.4238	3.4370
10	0.0066	-0.0034	0.0165	-3.4238	3.4370

Dissipation of chlormequat-Cl in aerobic Swiss pond water-silt loam sediment: water layer, nonlinear regression (MRID 46715227)



Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
Swiss Weiherhof-Tal pond water-silt loam sediment
Water layer
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 102.976}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.150043}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.98655295 Rsqr = 0.97328673 Adj Rsqr = 0.97137864

Standard Error of Estimate = 7.5078

	Coefficient	Std. Error	t	P
a	102.9765	3.3353	30.8752	<0.0001
b	0.1500	0.0171	8.7665	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	28752.0483	28752.0483	510.0841	<0.0001
Residual	14	789.1417	56.3673		
Total	15	29541.1900	1969.4127		

PRESS = 1268.3746

Durbin-Watson Statistic = 1.4713

Normality Test: K-S Statistic = 0.2396 Significance Level = 0.2770

Constant Variance Test: Passed (P = 0.2239)

Power of performed test with alpha = 0.0500: 1.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Weiherhof-Tal pond water-silt loam sediment
Water layer

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	102.9765	5.1235	0.6824	0.7617	0.7497
2	102.9765	3.1235	0.4160	0.4644	0.4510
3	99.1853	-1.2853	-0.1712	-0.1870	-0.1805
4	99.1853	-0.9853	-0.1312	-0.1434	-0.1383
5	88.6289	-2.3289	-0.3102	-0.3289	-0.3182
6	88.6289	-6.1289	-0.8163	-0.8656	-0.8574
7	76.2803	-2.8803	-0.3836	-0.4081	-0.3956
8	76.2803	-2.6803	-0.3570	-0.3797	-0.3678
9	36.0245	19.2755	2.5674	2.9962	4.8204
10	36.0245	4.5755	0.6094	0.7112	0.6981
11	12.6025	-12.0025	-1.5987	-1.7261	-1.8748
12	12.6025	-12.4025	-1.6520	-1.7837	-1.9552
13	1.1425	-0.7425	-0.0989	-0.0992	-0.0956
14	1.1425	-1.0425	-0.1389	-0.1392	-0.1343
15	0.0109	0.1891	0.0252	0.0252	0.0243
16	0.0109	0.0891	0.0119	0.0119	0.0114

Influence Diagnostics:

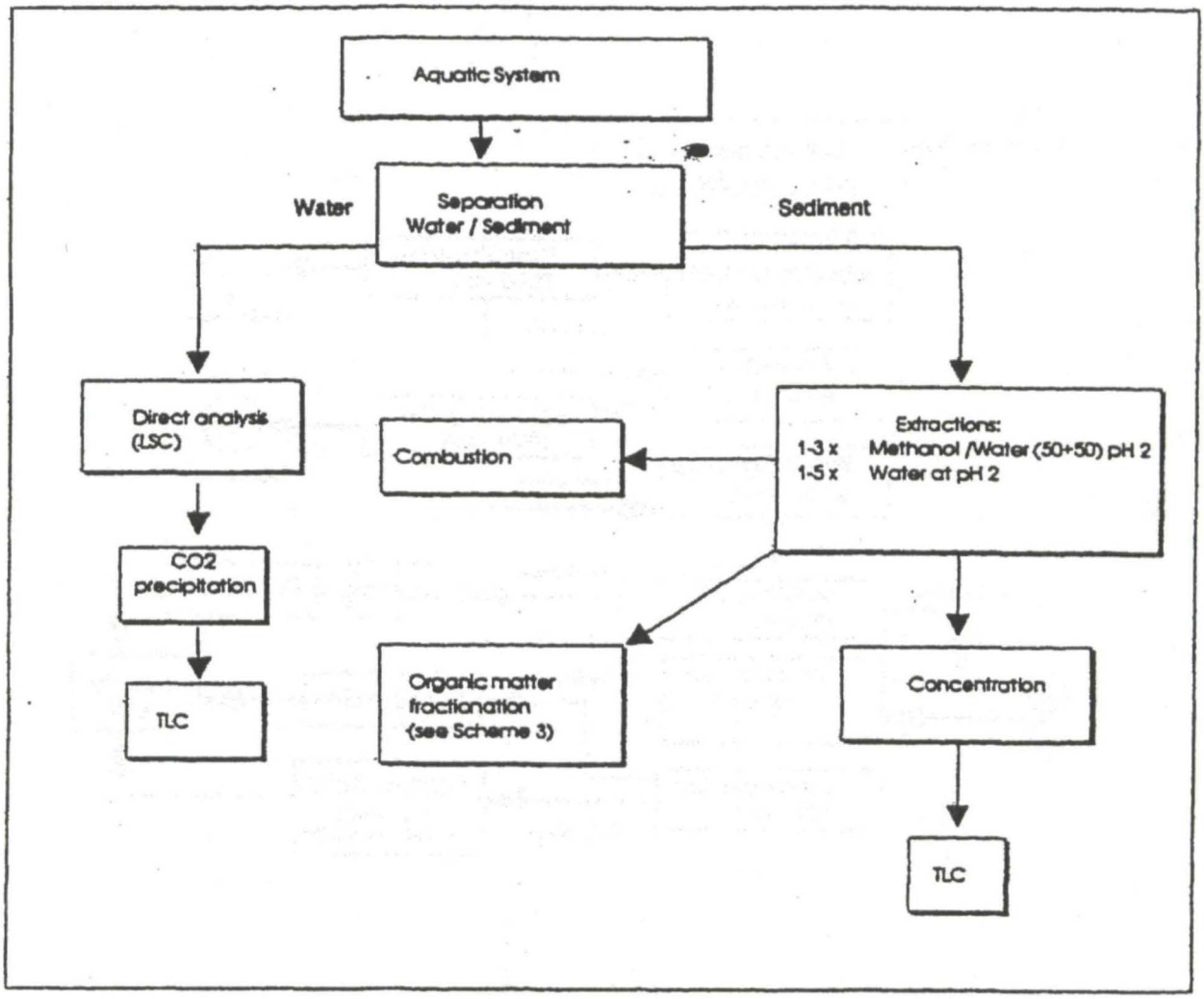
Row	Cook'sDist	Leverage	DFFITS
1	0.0713	0.1973	0.3717
2	0.0265	0.1973	0.2236
3	0.0034	0.1623	-0.0794
4	0.0020	0.1623	-0.0609
5	0.0067	0.1106	-0.1122
6	0.0466	0.1106	-0.3023
7	0.0109	0.1161	-0.1434
8	0.0095	0.1161	-0.1333
9	1.6248	0.2658	2.9002
10	0.0916	0.2658	0.4200
11	0.2470	0.1422	-0.7634
12	0.2637	0.1422	-0.7962
13	0.0000	0.0057	-0.0072
14	0.0001	0.0057	-0.0101
15	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000

Chemical: Chlormequat-chloride
PC: 018101
MRID 46715227
Guideline: 162-4
German Weiherhof-Tal pond water-silt loam sediment
Water layer
95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	102.9765	95.8231	110.1299	85.3564	120.5966
2	102.9765	95.8231	110.1299	85.3564	120.5966
3	99.1853	92.6976	105.6730	81.8248	116.5458
4	99.1853	92.6976	105.6730	81.8248	116.5458
5	88.6289	83.2742	93.9835	71.6593	105.5985
6	88.6289	83.2742	93.9835	71.6593	105.5985
7	76.2803	70.7937	81.7669	59.2686	93.2920
8	76.2803	70.7937	81.7669	59.2686	93.2920
9	36.0245	27.7231	44.3259	17.9080	54.1410
10	36.0245	27.7231	44.3259	17.9080	54.1410
11	12.6025	6.5298	18.6753	-4.6072	29.8122
12	12.6025	6.5298	18.6753	-4.6072	29.8122
13	1.1425	-0.0687	2.3537	-15.0057	17.2906
14	1.1425	-0.0687	2.3537	-15.0057	17.2906
15	0.0109	-0.0127	0.0346	-16.0918	16.1136
16	0.0109	-0.0127	0.0346	-16.0918	16.1136

Attachment 3: Transformation Pathway Presented by Registrant
Illustration of Test System
Analytical Pathway
Organic Matter Fractionation

Scheme 2: Analytical pathway.



Scheme 3: Organic matter fractionation.